

=> file reg

FILE 'REGISTRY' ENTERED AT 14:12:06 ON 20 JUN 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2001 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 19 JUN 2001 HIGHEST RN 342573-24-4
DICTIONARY FILE UPDATES: 19 JUN 2001 HIGHEST RN 342573-24-4

TSCA INFORMATION NOW CURRENT THROUGH January 11, 2001

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT
for details.

=> d his

(FILE 'HOME' ENTERED AT 12:19:56 ON 20 JUN 2001)

FILE 'LREGISTRY' ENTERED AT 12:21:16 ON 20 JUN 2001

L1 STR
L2 STR L1
L3 STR
L4 STR
L5 STR L3

FILE 'REGISTRY' ENTERED AT 13:28:53 ON 20 JUN 2001

L6 0 S L2 OR L5 OR L4

FILE 'LREGISTRY' ENTERED AT 13:29:11 ON 20 JUN 2001

L7 STR

FILE 'REGISTRY' ENTERED AT 13:39:29 ON 20 JUN 2001

L8 0 S L7

FILE 'LREGISTRY' ENTERED AT 13:39:56 ON 20 JUN 2001

L9 STR L7

FILE 'REGISTRY' ENTERED AT 13:40:58 ON 20 JUN 2001

L10 18 S L9
L11 283 S L9 FUL
SAV L11 PAD859/A
L12 0 S (L2 OR L5 OR L4) SSS SAM SUB=L11
L13 2 S (L2 OR L5 OR L4) SSS FUL SUB=L11
SAV L13 PAD859A/A
L14 0 S L7 SSS SAM SUB=L11
L15 5 S L7 SSS FUL SUB=L11
SAV L15 PAD859B/A

L16 5 S L15 NOT L13

FILE 'HCA' ENTERED AT 13:48:44 ON 20 JUN 2001

L17 2 S L13
 L18 8 S L15
 L19 132 S L11
 L20 75174 S (CVD OR (CHEMICAL? OR CHEM) (2A) (VAPOR? OR VAPOUR?) (2A) D
 L21 19 S L19 AND L20
 L22 8 S L18 NOT L17
 L23 19 S L21 NOT (L17 OR L22)

FILE 'REGISTRY' ENTERED AT 14:12:06 ON 20 JUN 2001

=> d l11 que stat

L9 STR

		24		27		25	
		G2		F		C	
		⋈		⋈		⋈	
Ta~G1	NH~G2	N~G2	@14 Ak~F	@17 Si~C			Ak @20
2 3	@5 6	@9 10	15	18			
			⋈	⋈			
			F	C			
			28	26			

VAR G1=NH2/5/9

VAR G2=20/PH/14/17

NODE ATTRIBUTES:

NSPEC IS RC AT 2

NSPEC IS RC AT 18

NSPEC IS RC AT 25

NSPEC IS RC AT 26

CONNECT IS E1 RC AT 20

DEFAULT MLEVEL IS ATOM

GGCAT IS SAT AT 20

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M1-X4 C AT 20

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L11 283 SEA FILE=REGISTRY SSS FUL L9

100.0% PROCESSED 10689 ITERATIONS

283 ANSWERS

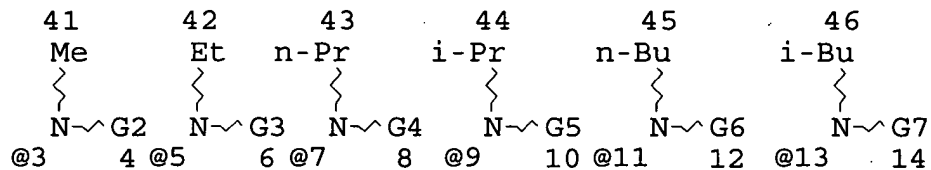
SEARCH TIME: 00.00.01

=> d l13 que stat

L2 STR

Ta \wedge G1

1 2



VAR G1=3/5/7/9/11/13

VAR G2=ET/N-PR/I-PR/N-BU/I-BU/S-BU/T-BU

VAR G3=ME/N-PR/I-PR/N-BU/I-BU/S-BU/T-BU

VAR G4=ME/ET/I-PR/N-BU/I-BU/S-BU/T-BU

VAR G5=ME/ET/N-PR/N-BU/I-BU/S-BU/T-BU

VAR G6=ME/ET/N-PR/I-PR/I-BU/S-BU/T-BU

VAR G7=ME/ET/N-PR/I-PR/N-BU/S-BU/T-BU

NODE ATTRIBUTES:

CONNECT IS E5 C AT 1

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L4 STR



VAR G1=20/PH/18

NODE ATTRIBUTES:

NSPEC IS RC AT 22

NSPEC IS RC AT 23

NSPEC IS RC AT 24

CONNECT IS E1 RC AT 20

CONNECT IS E5 C AT 27

DEFAULT MLEVEL IS ATOM

GGCAT IS SAT AT 20

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M1-X4 C AT 20

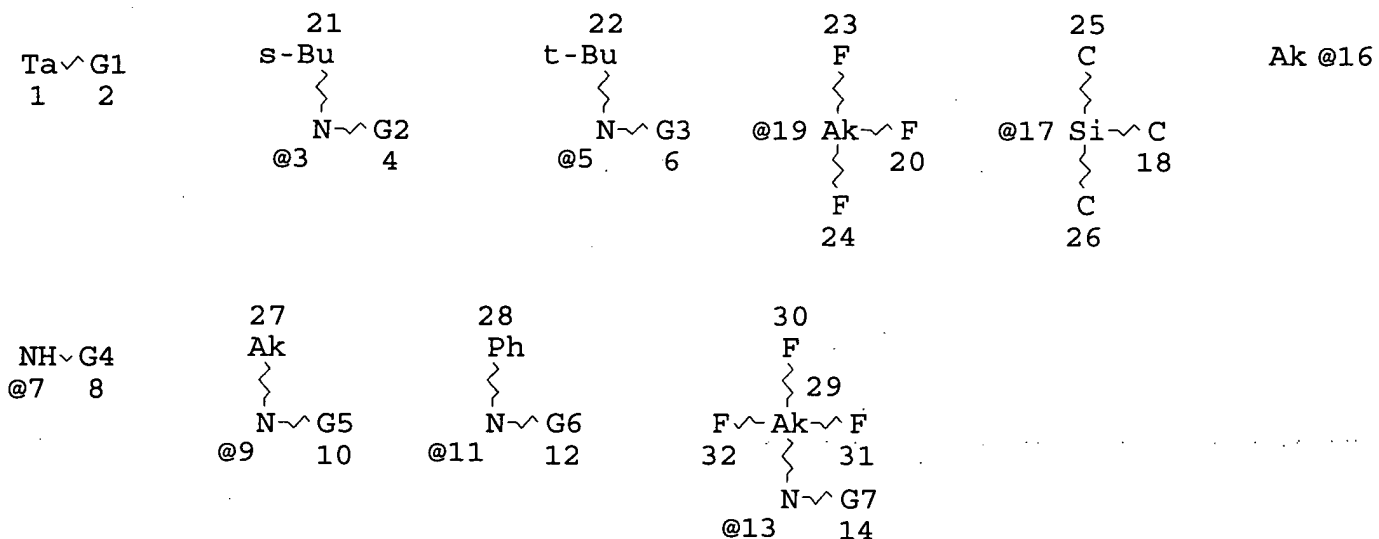
GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 12

STEREO ATTRIBUTES: NONE

L5 STR



VAR G1=3/5/7/9/11/13

VAR G2=ME/ET/N-PR/I-PR/N-BU/I-BU/T-BU

VAR G3=ME/ET/N-PR/I-PR/N-BU/I-BU/S-BU

VAR G4=ME/ET/N-PR/I-PR/N-BU/I-BU/S-BU/PH/19/17

VAR G5=PH/19/17

VAR G6=16/19/17

VAR G7=16/PH/17

NODE ATTRIBUTES:

NSPEC IS RC AT 18

NSPEC IS RC AT 25

NSPEC IS RC AT 26

CONNECT IS E5 C AT 1

CONNECT IS E1 RC AT 16

CONNECT IS E1 RC AT 27

DEFAULT MLEVEL IS ATOM

GGCAT IS SAT AT 16

GGCAT IS SAT AT 27

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS M1-X4 C AT 16

ECOUNT IS M1-X4 C AT 27

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 31

STEREO ATTRIBUTES: NONE

```
VAR G1=NH2/5/9
VAR G2=20/PH/14/17
```

NODE ATTRIBUTES:

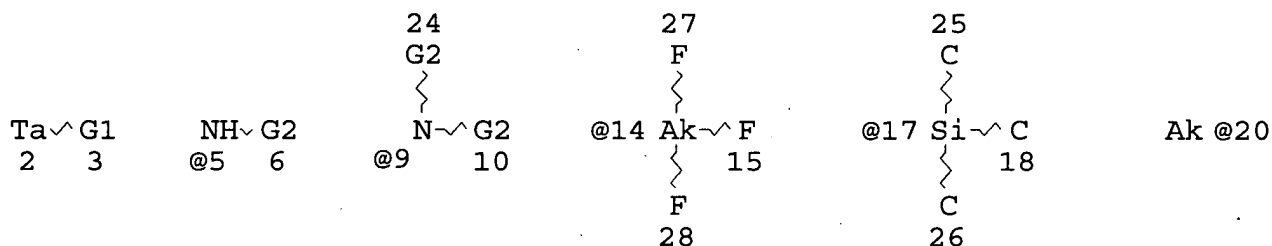
NSPEC IS RC AT 18
 NSPEC IS RC AT 25
 NSPEC IS RC AT 26
 CONNECT IS E1 RC AT 20
 DEFAULT MLEVEL IS ATOM
 GGCAT IS SAT AT 20
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS M1-X4 C AT 20

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L9 STR



VAR G1=NH2/5/9

VAR G2=20/PH/14/17

NODE ATTRIBUTES:

NSPEC IS RC AT 2
 NSPEC IS RC AT 18
 NSPEC IS RC AT 25
 NSPEC IS RC AT 26
 CONNECT IS E1 RC AT 20
 DEFAULT MLEVEL IS ATOM
 GGCAT IS SAT AT 20
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS M1-X4 C AT 20

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L11 283 SEA FILE=REGISTRY SSS FUL L9

L15 5 SEA FILE=REGISTRY SUB=L11 SSS FUL L7

100.0% PROCESSED 283 ITERATIONS (5 INCOMPLETE)

5 ANSWERS

SEARCH TIME: 00.00.02

=> file hca

FILE 'HCA' ENTERED AT 14:13:02 ON 20 JUN 2001
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2001 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE COVERS 1947 - 14 Jun 2001 VOL 134 ISS 26
FILE LAST UPDATED: 14 Jun 2001 (20010614/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REGISTRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

The HCA file now provides online access to patents and literature covered in CA from 1947 to the present. On April 22, 2001, bibliographic information and abstracts were added for over 2.2 million references published in CA from 1947 to 1966.

The CA Lexicon is now available in the Controlled Term (/CT) field. Enter HELP LEXICON for full details.

Attention, the CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

=> d l17 1-2 ibib abs hitstr hitind

L17 ANSWER 1 OF 2 HCA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 118:102151 HCA
TITLE: Methane vs benzene activation via transient
tantalum amido-imido complex
tert-Bu₃SiNHTa(:NSiBu₃-tert)₂: structure of
(py)₂MeTa(:NSiBu₃-tert)₂
AUTHOR(S): Schaller, Christopher P.; Wolczanski, Peter T.
CORPORATE SOURCE: Dep. Chem., Cornell Univ., Ithaca, NY, 14853,
USA
SOURCE: Inorg. Chem. (1993), 32(2), 131-44
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal

gnd

LANGUAGE: English

OTHER SOURCE(S): CASREACT 118:102151

AB Addn. of Me_3TaCl_2 to 2.0 equiv of LiNHSiR_3 ($\text{R} = \text{CMe}_3$ throughout this abstr.) in hexanes resulted in CH_4 and $(\text{R}_3\text{SiNH})\text{Me}_2\text{Ta}:\text{NSiR}_3$ (1, 63%). Thermolysis of 1 in benzene resulted in disproportionation, but in pyridine and THF, $\text{L}_2\text{MeTa}(:\text{NSiR}_3)_2$ ($\text{L} = \text{py}$, $2(\text{py})_2$, 68%; THF, $2(\text{THF})_2$, 13%) and MeH were produced. The bis adduct $2(\text{py})_2$ is considered to form via 1,2-MeH-elimination from $(\text{R}_3\text{SiNH})\text{Me}_2(\text{py})\text{Ta}:\text{NSiR}_3$ (1-py), which is obtained from 1 and pyridine at 25.degree.. ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of $2(\text{py})_2$ manifested equiv. pyridines, but an x-ray structure detn. revealed a trigonal bipyramidal, pseudo-Cs stereoisomer with an axial Me group and equatorial imides that reflects the steric requirements of the bulky R_3SiN units. Rather long Ta:N bond distances (1.810 (13) and 1.819 (13) .ANG.) support electronic arguments suggesting the imides donate a max. of 6 electrons to the metal center. Addn. of TaCl_5 to 4.0 equiv of LiNHSiR_3 in Et_2O at -78.degree. afforded $(\text{R}_3\text{SiNH})_2\text{ClTa}:\text{NSiR}_3$ (3-Cl) and R_3SiNH_2 . Alkylation of 3-Cl with AlMe_3 (hexanes), PhLi (Et_2O /hexanes), PhCH_2K (toluene), and RCH_2Li (Et_2O) provided $(\text{R}_3\text{SiNH})_2\text{RTa}:\text{NSiR}_3$ ($\text{R} = \text{Me}$, 3-Me, 78%; Ph, 3-Ph, 64%; CH_2Ph , 3- CH_2Ph , 51%; CH_2R , 3- CH_2R , 39%). Addn. of R_3SiNH_2 or R_3SiOH to 1 yielded 3-Me or $(\text{R}_3\text{SiNH})(\text{R}_3\text{SiO})\text{MeTa}:\text{NSiR}_3$ (5-Me, 52%) and CH_4 . Thermolysis of 3-R effected 1,2-RH-elimination to form transient $(\text{R}_3\text{SiNH})\text{Ta}(:\text{NSiR}_3)_2$ (4), a species capable of adding C-H bonds across one imido linkage. Moderate rates of elimination from 3-R could be obtained only at 182.8 (4).degree.. Ground-state information was obtained via the approach to equil. of 3-Ph and CH_4 , but observation of a p-ditantalum Ph deriv., $[(\text{R}_3\text{SiNH})_2\text{Ta}:\text{NSiR}_3]_2(\mu\text{..eta.1,eta.1-1,4-C}_6\text{H}_4)((3)2\text{C}_6\text{H}_4)$ complicated the measurement. Simulation of the approach to equil. yielded rate consts. consistent with the previously measured 1,2-RH-elimination rates and showed that 3-Me, 3-Ph, and $(3)2\text{C}_6\text{H}_4$ possess relatively similar ground-state free energies. Equilibration of 3- CH_2Ph to aryl complexes $(\text{R}_3\text{SiNH})_2(\text{C}_6\text{H}_4\text{Me})\text{Ta}:\text{NSiR}_3$ (3- $\text{C}_6\text{H}_4\text{Me})$ in toluene at 182.8 (4).degree. gave similar results. The data portray differing 1,2-RH-elimination rates that result from significant transition state energy differences, ruling out a late transition state despite a rough correlation of rate with the C-H bond strength of the eliminated alkane/arene. The implications of these measurements, including the possibility of d0 alkane or arene complexes as intermediates and differences in tantalum-carbon bond strengths, are discussed in detail.

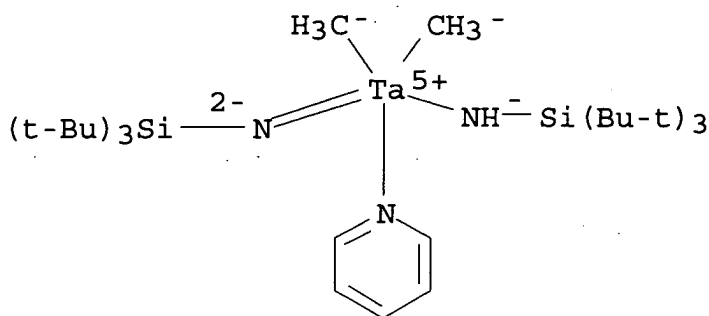
IT 146128-74-7P

(prepn. of)

RN 146128-74-7 HCA

CN Tantalum, dimethyl(pyridine)[1,1,1-tris(1,1-dimethylethyl)silanaminato][1,1,1-tris(1,1-dimethylethyl)silanaminato(2-)]- (9CI) (CA INDEX NAME)

*center group has no Si or N
no use taught
only 3(NRR)
groups
not 5*



CC 29-10 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 22, 75

IT 145674-28-8P 145674-29-9P 145702-63-2P **146128-74-7P**
146128-76-9P

(prepn. of)

L17 ANSWER 2 OF 2 HCA COPYRIGHT 2001 ACS

ACCESSION NUMBER: 108:86837 HCA

TITLE: Synthesis and structure of niobium(V) and tantalum(V) organoimido compounds containing 2,6-diphenylphenoxide ligation

AUTHOR(S): Chesnut, Robert W.; Fanwick, Phillip E.; Rothwell, Ian P.

CORPORATE SOURCE: Dep. Chem., Purdue Univ., West Lafayette, IN, 47905, USA

SOURCE: Inorg. Chem. (1988), 27(4), 752-4

CODEN: INOCAJ; ISSN: 0020-1669

DOCUMENT TYPE: Journal

LANGUAGE: English

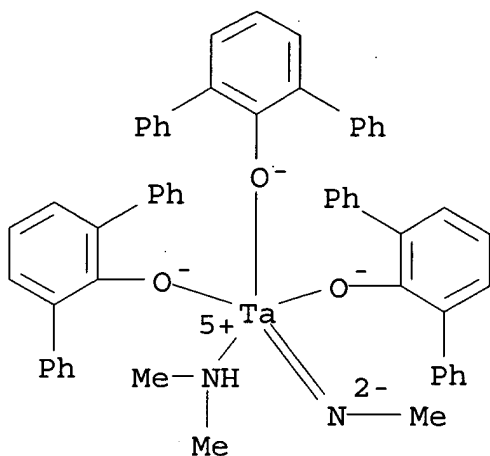
AB The addn. of 3 equiv of 2,6-diphenylphenol (HOAr-2,6Ph₂) to a toluene soln. of M(NMe₂)₅ (M = Nb, Ta) gave, on warming, M(OAr-2,6Ph₂)₃(NMe)(NHMe₂) (I). A single crystal diffraction study of I (M = Nb) confirmed the stoichiometry and showed a geometry about the metal center best described as trigonal bipyramidal with an essentially linear Nb:NMe bond. As expected the Nb:NMe bond of 1.720(5) Å is dramatically shorter than that to the amine ligand, 2.326(6) Å. I (M = Nb) is orthorhombic with a = 10.808(2), b 19.499(4), c = 21.801(3) Å, Z = 4, d.(calcd.) = 1.305 g cm⁻³ in space group P2₁2₁2₁.

IT **112347-60-1P**

(prepn. of)

RN 112347-60-1 HCA

CN Tantalum, [methanaminato(2-)](N-methylmethanamine)tris([1,1':3',1''-terphenyl]-2'-olato)-, (TB-5-12)- (9CI) (CA INDEX NAME)



organos Ta

CC 78-7 (Inorganic Chemicals and Reactions)
 Section cross-reference(s): 75
 IT 112347-60-1P
 (prepn. of)

=> d 122 1-8 cbib abs hitstr hitind

L22 ANSWER 1 OF 8 HCA COPYRIGHT 2001 ACS

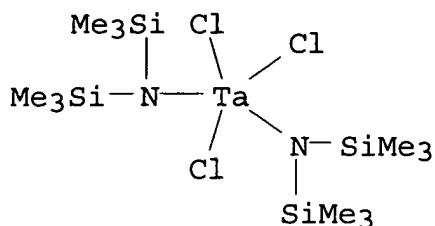
125:184166 Synthesis and Structural Characterization of Tantalum(IV) Amido Compounds. Suh, Seigi; Hoffman, David M. (Department of Chemistry, University of Houston, Houston, TX, 77204, USA). Inorg. Chem., 35(17), 5015-5018 (English) 1996. CODEN: INOCAJ. ISSN: 0020-1669.

AB Ta(IV) amido complexes were synthesized from Ta(V) precursors. Ta(N(SiMe3)2)2Cl3 reacts with Na/Hg to give Ta(N(SiMe3)2)2Cl2, and Ta(NEt2)2Cl3 reacts with LiNPh2 and Na/Hg to yield Ta(NPh2)2(NEt2)2. Ta(N(SiMe3)2)2Ph2 was prepd. by reacting Ta(N(SiMe3)2)2Cl2 with LiPh. Attempts to prep. other organometallic derivs. failed to yield clean products. X-ray crystallog. studies show that Ta(N(SiMe3)2)2Cl2, Ta(N(SiMe3)2)2Ph2, and Ta(NPh2)2(NEt2)2 have distorted tetrahedral geometries.

IT 71616-54-1, Trichlorobis(bis(trimethylsilyl)amido)tantalum
 (for prepn. of tantalum 4 amido complexes)

RN 71616-54-1 HCA

CN Tantalum, trichlorobis[1,1,1-trimethyl-N-(trimethylsilyl)silanaminato]-, (SP-5-11)- (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 29, 75

IT 591-51-5, Phenyllithium 5856-89-3, Lithium diphenylamide
71616-54-1, Trichlorobis(bis(trimethylsilyl)amido)tantalum
 99449-55-5

(for prepn. of tantalum 4 amido complexes)

L22 ANSWER 2 OF 8 HCA COPYRIGHT 2001 ACS

119:61653 Syntheses and crystal structure of tantalum(IV) amido and imido halide complexes. Hoffman, David M.; Suh, Seigi (Dep. Chem., Univ. Houston, Houston, TX, 77204, USA). J. Chem. Soc., Chem. Commun. (8), 714-15 (English) 1993. CODEN: JCCCAT. ISSN: 0022-4936.

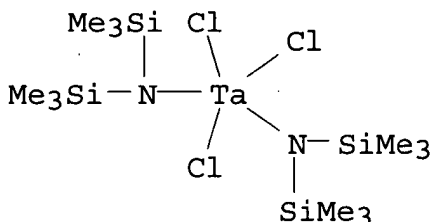
AB The syntheses and crystal structures of monomeric Ta(IV) amido halide and dimeric Ta(IV) imido halide complexes are reported. Ta[N(SiMe₃)₂]₂Cl₃ was reduced by Na/Hg to give Ta[N(SiMe₃)₂]₂Cl₂ (I). Ta(NSiMe₃)[N(SiMe₃)₂Cl₂(THF)] was similarly reduced to give {Ta(.mu.-NSiMe₃)[N(SiMe₃)₂Cl]}₂ (II). I and II were characterized by elemental anal., NMR and IR spectrometries, and x-ray crystallog. I has a severely distorted tetrahedral geometry. II has an edge-shared tetrahedral structure and a Ta-Ta distance of 2.621(1) .ANG..

IT **71616-54-1**

(redn. of, by sodium amalgam)

RN 71616-54-1 HCA

CN Tantalum, trichlorobis[1,1,1-trimethyl-N-(trimethylsilyl)silanaminato]-, (SP-5-11)- (9CI) (CA INDEX NAME)



3(Cl)

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 75

IT **71616-54-1** 134588-18-4

(redn. of, by sodium amalgam)

L22 ANSWER 3 OF 8 HCA COPYRIGHT 2001 ACS

115:20938 Organoimidotantalum(V) complexes containing halide, dialkylamide, monoalkylamide, alkoxide, aryloxy, trialkylphosphine and tetrahydrofuran ligands. Crystal structures of $[\{Ta(\mu\text{-Cl})Cl(NSiMe_3)[N(SiMe_3)_2]\}_2]$ and $[\{Ta(\mu\text{-OMe})(OMe)(NSiMe_3)[N(SiMe_3)_2]\}_2]$. Bradley, Donald C.; Hursthouse, Michael B.; Howes, Andrew J.; Jelfs, Alasdair N. de M.; Runnacles, John D.; Thornton-Pett, Mark (Dep. Chem., Queen Mary and Westfield Coll., London, E1 4NS, UK). J. Chem. Soc., Dalton Trans. (150th Anniv. Celebration Issue), 841-7 (English) 1991. CODEN: JCDBTBI. ISSN: 0300-9246.

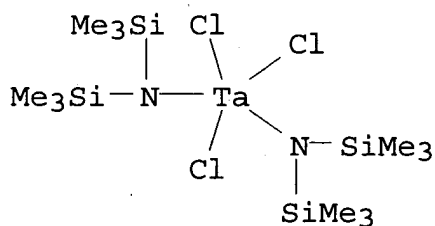
AB By means of various reactions $[TaCl_3\{N(SiMe_3)_2\}_2]$ was converted into the $[\{Ta(\mu\text{-X})X(NSiMe_3)[N(SiMe_3)_2]\}_2]$ (I: X = Cl, I), $[TaCl_2(NSiMe_3)\{N(SiMe_3)_2\}(THF)]$, $[Ta(NEt)(NHet)\{N(SiMe_3)_2\}_2]$, and $[Ta(NCMe_3)(NHet)\{N(SiMe_3)_2\}_2]$. From I (X = Cl) $[Ta(NSiMe_3)\{NSiMe_3\}_2](NHCMe_3)_2]$, $[Ta(NSiMe_3)\{N(SiMe_3)_2\}(OCMe_3)_2]$, and $[\{Ta(\mu\text{-OMe})(OMe)(NSiMe_3)[N(SiMe_3)_2]\}_2]$ (II) were obtained and from $[TaCl_3(OC_6H_2Me(CMe_3)_2)_2]$, $[Ta(NEt)(NHet)(OC_6H_2Me(CMe_3)_2)_2]$, $[Ta(NCH_2CMe_3)(NHCH_2CMe_3)(OC_6H_2Me(CMe_3)_2)_2]$, and $[Ta(NCMe_3)(NHCMe_3)(OCH_2Me(CMe_3)_2)_2]$ were prepd. $[TaCl_3(NPh)(PEt_3)_2]$ and $[TaCl_3(NPh)(PEt_2Ph)_2]$ were prepd. from reaction involving $NHPh(SiMe_3)$ and $TaCl_5$ in the presence of trialkylphosphines. All of these new compds. were characterized by NMR, IR, and mass spectra and I (X = Cl) and II were structurally characterized by single-crystal x-ray crystallog. I (X = Cl) is triclinic, space group P $\bar{1}$, Z = 1, R = 0.035, R₁ = 0.040; II is monoclinic, space group P2₁/n, Z = 2, R = 0.057, R₁ = 0.051.

IT 71616-54-1

(reaction of, with iodotrimethylsilane and THF and ethylamide)

RN 71616-54-1 HCA

CN Tantalum, trichlorobis[1,1,1-trimethyl-N-(trimethylsilyl)silanaminato]-, (SP-5-11)- (9CI) (CA INDEX NAME)



Not used given

CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 75

IT 71616-54-1

(reaction of, with iodotrimethylsilane and THF and ethylamide)

L22 ANSWER 4 OF 8 HCA COPYRIGHT 2001 ACS

101:182554 Organoimido complexes of tantalum(V). Preparation and x-ray crystal structure of bis[bis(trimethylsilyl)amido]chloro(tert-

butylimido)tantalum(V) and bis[bis(trimethylsilyl)amido]-di-.mu.-bromodibromobis(trimethylsilylimido)ditantalum(V). Bradley, Donald C.; Hursthouse, Michael B.; Malik, K. M. Abdul; Nielson, Alistair J.; Chota Vuru, George B. (Dep. Chem., Queen Mary Coll., London, E1 4NS, UK). J. Chem. Soc., Dalton Trans. (6), 1069-72 (English) 1984. CODEN: JCDBTBI. ISSN: 0300-9246.

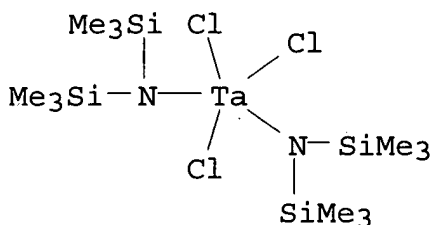
AB Reaction of $\text{TaCl}_3[\text{N}(\text{SiMe}_3)_2]_2$ (I) with LiNHCM_3 in pentane for 15 h gave 71% $\text{TaCl}(\text{NCMe}_3)[\text{N}(\text{SiMe}_3)_2]_2$ (II). I with Me_3SiBr in refluxing PhMe for 6 h gave 25% $[\text{TaBr}_2(\text{NSiMe}_3)[\text{N}(\text{SiMe}_3)_2]]_2$ (III), a centrosym. 5-coordinated dimer. II is monoclinic, space group $P2_1/n$, with a 12.343(2), b 19.089(3), c 12.135(3) .ANG., .beta. 94.98(3).degree., $Z = 4$, $d.(\text{calcd.}) = 1.42 \text{ g cm}^{-3}$, $R = 0.041$. III is triclinic, space group $P_{hivn}.1$, with a 9.254(4), b 9.340(4), c 12.287(5), .alpha. 87.57(4), .beta. 84.04(4), .gamma. 102.30(4).degree., $Z = 1$, $d.(\text{calcd.}) = 1.905 \text{ g cm}^{-3}$, $R = 0.053$. Treatment of III with pyridine or PMe_3 cleaved the unsym. Br bridge to give $\text{TaBr}_2(\text{NSiMe}_3)[\text{N}(\text{SiMe}_3)_2]\text{L}$ ($\text{L} = \text{py}, \text{PMe}_3$). Reaction of I with $\text{NaS}_2\text{CNMe}_2$ gave $\text{Ta}(\text{NSiMe}_3)(\text{S}_2\text{CNMe}_2)_3(\text{CH}_2\text{Cl}_2)$, which may involve a 7-coordinated Ta imido complex.

IT 71616-54-1

(substitution reactions of, imido complexes by)

RN 71616-54-1 HCA

CN Tantalum, trichlorobis[1,1,1-trimethyl-N-(trimethylsilyl)silanaminato]-, (SP-5-11)- (9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 75

IT 71616-54-1

(substitution reactions of, imido complexes by)

L22 ANSWER 5 OF 8 HCA COPYRIGHT 2001 ACS

93:8260 The preparation, characterization and crystal and molecular structure of bis(bis(trimethylsilyl)amido)trichlorotantalum(V). Bradley, Donald C.; Hursthouse, Michael B.; Malik, K. M. Abdul; Vuru, George B. C. (Dep. Chem., Queen Mary Coll., London, E1 4NS, Engl.). Inorg. Chim. Acta, 44(1), L5-L6 (English) 1980. CODEN: ICHAA3. ISSN: 0020-1693.

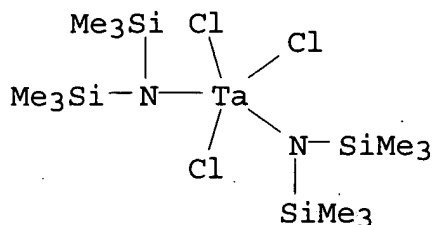
AB In the reaction with $\text{LiN}(\text{SiMe}_3)_2$, TaCl_5 underwent only disubstitution to give $\text{TaCl}_3[\text{N}(\text{SiMe}_3)_2]_2$ (I), irresp. of the $\text{LiN}(\text{SiMe}_3)_2$ - TaCl_5 mol ratio (1-5) in pentane. Structure detns. of I indicated that it had a distorted trigonal bipyramidal structure in which the bulky $\text{N}(\text{SiMe}_3)_2$ groups occupied equatorial sites.

IT 71616-54-1P

(prepn. and structure of)

RN 71616-54-1 HCA

CN Tantalum, trichlorobis[1,1,1-trimethyl-N-(trimethylsilyl)silanaminato]-, (SP-5-11)- (9CI) (CA INDEX NAME)



CC 29-10 (Organometallic and Organometalloidal Compounds)

IT 71616-54-1P

(prepn. and structure of)

L22 ANSWER 6 OF 8 HCA COPYRIGHT 2001 ACS

93:8233 A convenient preparation of metal pseudohalide compounds.
 Andersen, Richard A. (Chem. Dep., Univ. California, Berkeley, CA, 94720, USA). Inorg. Nucl. Chem. Lett., 16(1), 31-2 (English) 1980.
 CODEN: INUCAF. ISSN: 0020-1650.

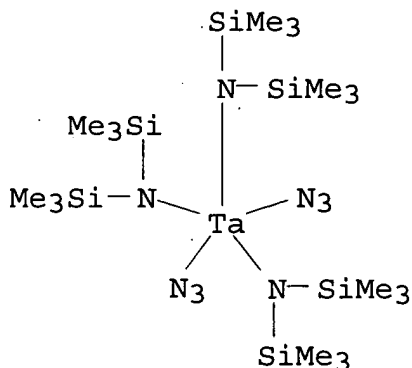
AB A reaction of [(Me₃Si)₂N]3HfCl with Me₃SiX gave [(Me₃Si)₂N]3HfX (X = Br, I, N₃, CN), quant. [(Me₃Si)₂N]2Ta(N₃)₃ was similarly prepd.

IT 73830-77-0P

(prepn. of)

RN 73830-77-0 HCA

CN Tantalum, diazidotris[1,1,1-trimethyl-N-(trimethylsilyl)silanaminato]- (9CI) (CA INDEX NAME)



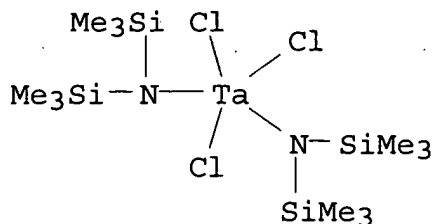
IT 71616-54-1

(reaction of, with trimethylsilyl azide)

RN 71616-54-1 HCA

CN Tantalum, trichlorobis[1,1,1-trimethyl-N-

(trimethylsilyl)silanaminato]-, (SP-5-11)- (9CI) (CA INDEX NAME)



CC 29-6 (Organometallic and Organometalloidal Compounds)

IT 73830-74-7P 73830-75-8P 73830-76-9P **73830-77-0P**
73841-10-8P

(prepn. of)

IT **71616-54-1**

(reaction of, with trimethylsilyl azide)

L22 ANSWER 7 OF 8 HCA COPYRIGHT 2001 ACS

91:211518 Trimethylbis[bis(trimethylsilyl)amido]tantalum(V) and [(trimethylsilyl)methyl][trimethylsilylmethylidene]bis[bis(trimethylsilyl)amido]tantalum(V). Andersen, Richard A. (Dep. Chem., Univ. California, Berkeley, CA, 94720, USA). Inorg. Chem., 18(12), 3622-3 (English) 1979. CODEN: INOCAJ. ISSN: 0020-1669.

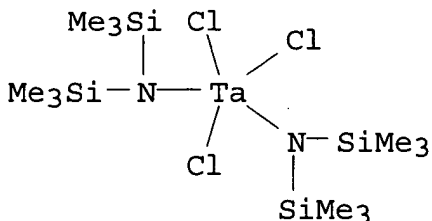
AB Bis(hexamethyldisilylamido)trichlorotantalum, from Na hexamethyldisilylamide and TaCl₅, yields Me₃Ta[N(SiMe₃)₂]₂ upon reaction with MeLi. The structure of this five-coordinate species is most reasonably described as a square pyramid with hexamethyldisilylamido ligands trans to each other and cis to the 3 Me-Ta groups. The carbene complex, (Me₃SiCH₂)(Me₃SiCH)Ta[N(SiMe₃)₂]₂, is formed from the trichloride and Me₃SiCH₂Li.

IT **71616-54-1P 71616-55-2P**

(prepn. of)

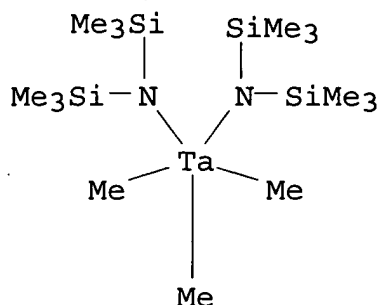
RN 71616-54-1 HCA

CN Tantalum, trichlorobis[1,1,1-trimethyl-N-(trimethylsilyl)silanaminato]-, (SP-5-11)- (9CI) (CA INDEX NAME)



RN 71616-55-2 HCA

CN Tantalum, trimethylbis[1,1,1-trimethyl-N-(trimethylsilyl)silanaminato]-, (SP-5-21)- (9CI) (CA INDEX NAME)



2(N⁺)
3(Me)

CC 29-10 (Organometallic and Organometalloidal Compounds)
IT 71616-54-1P 71616-55-2P 71616-56-3P
(prepn. of)

L22 ANSWER 8 OF 8 HCA COPYRIGHT 2001 ACS

81:32725 Complexes of tantalum and antimony pentafluorides with dimethyl ether and trimethylamine. Brownstein, S.; Farrall, Marjorie J. (Div. Chem., Natl. Res. Counc. Canada, Ottawa, Ont., Can.). Can. J. Chem., 52(10), 1958-65 (English) 1974. CODEN: CJCHAG.

AB TaF5 forms 1:1 and 1:2 complexes with Me2O and Me3N. SbF5 forms 2:1 and 1:1 complexes with Me2O and Me3N. The rates of exchange of terminal and equatorial fluorines in the 1:1 TaF5-Me2O adduct are measured.

IT 53129-67-2
(exchange of fluorine in, NMR in relation to)

RN 53129-67-2 HCA

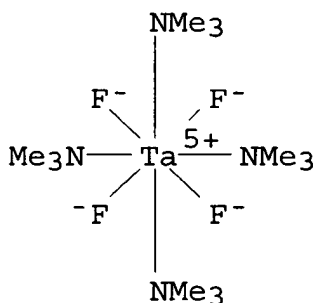
CN Tantalum(1+), tetrakis(N,N-dimethylmethanamine)tetrafluoro-,
(OC-6-11)-hexafluorotantalate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 53129-66-1

CMF C12 H36 F4 N4 Ta

CCI CCS



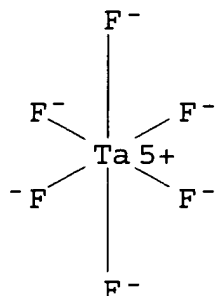
CM 2

CRN 16918-70-0

CMF F6 Ta

CCI CCS

CDES 7:OC-6-11



CC 78-9 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 67

IT 12122-12-2 53129-63-8 53129-65-0 **53129-67-2**

53129-68-3 53129-69-4 53129-70-7

(exchange of fluorine in, NMR in relation to)

=> d 123 1-19 cbib abs hitstr hitind

L23 ANSWER 1 OF 19 HCA COPYRIGHT 2001 ACS

134:374292 Tantalum-carbon thin films for low-resistivity barrier layers and their manufacture by MOCVD. Nakamura, Satoshi; Komatsu, Takashi; Higuchi, Yasushi; Nagano, Kenzo; Taguma, Yasuhiro (ULVC Japan, Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2001131746 A2 20010515, 6 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1999-318244 19991109.

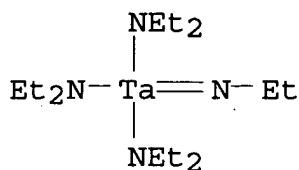
AB The process comprises deposition of C-rich layers on substrates by **MOCVD** and plasma exposure of the layers while applying bias potential on the substrates to give Ta-C layers with resistivity 350-2000 .mu..OMEGA.cm. The **MOCVD** sources may be alkylaminotantalum compds.

IT **67313-80-8**

(source; manuf. of Ta-C thin films for low-resistivity barrier layers by **MOCVD** and followed plasma exposure)

RN 67313-80-8 HCA

CN Tantalum, [ethanaminato(2-)]tris(N-ethylethanaminato)-, (T-4)- (9CI)
(CA INDEX NAME)



- IC ICM C23C016-32
ICS H01L021-285; H01L021-3205
- CC 75-1 (Crystallography and Liquid Crystals)
Section cross-reference(s): 76
- ST tantalum carbon barrier layer low resistivity; MOCVD
plasma annealing tantalum carbon layer; alkylaminotantalum
MOCVD tantalum carbon barrier layer
- IT Electric conductors
(barrier layers; manuf. of Ta-C thin films for low-resistivity
barrier layers by **MOCVD** and followed plasma exposure)
- IT Bias potential
Plasma
(manuf. of Ta-C thin films for low-resistivity barrier layers by
MOCVD and followed plasma exposure)
- IT Vapor deposition process
(metalorg.; manuf. of Ta-C thin films for low-resistivity barrier
layers by **MOCVD** and followed plasma exposure)
- IT Annealing
(plasma; manuf. of Ta-C thin films for low-resistivity barrier
layers by **MOCVD** and followed plasma exposure)
- IT 164992-28-3P
(manuf. of Ta-C thin films for low-resistivity barrier layers by
MOCVD and followed plasma exposure)
- IT 7439-90-9, Krypton, uses 7440-37-1, Argon, uses 7440-63-3,
Xenon, uses 7727-37-9, Nitrogen, uses
(plasma contg.; manuf. of Ta-C thin films for low-resistivity
barrier layers by **MOCVD** and followed plasma exposure)
- IT **67313-80-8**
(source; manuf. of Ta-C thin films for low-resistivity barrier
layers by **MOCVD** and followed plasma exposure)

L23 ANSWER 2 OF 19 HCA COPYRIGHT 2001 ACS

134:319599 Method for fabricating gate oxide layer for a semiconductor device. Huang, Kuo-Tai; Huang, Michael W. C.; Yew, Tri-Rung (United Microelectronics Corp., Taiwan). U.S. US 6221712 B1 20010424, 8 pp. (English). CODEN: USXXAM. APPLICATION: US 1999-385805 19990830.

AB A method is provided for fabricating a gate structure. The method involves providing a substrate, followed by forming a nitride region on a surface of the substrate. With a Ta-based org. compd. and a Ti-based org. compd. serving as precursors, an metalorg. **CVD** (**MOCVD**) is performed, so that a Ta₂-xTi_xO₅ dielec. layer is formed on the substrate. A barrier layer, a conducting layer, and an anti-reflection (AR) layer are then formed in sequence on the Ta₂-xTi_xO₅ dielec. layer. Subsequently, the AR layer, the

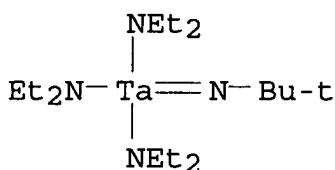
conducting layer, the barrier layer, and the Ta₂-xTi_xO₅ dielec. layer are defined to form a gate structure on the substrate of the nitride region. The Ta-based org. compd. in this case may include a Ta-alkoxide compd., whereas the Ti-based org. compd. may include a Ti-alkoxide compd. or a Ti-amide compd.

* IT 169896-41-7

(vapor deposition precursor; method for fabricating gate oxide layer for a semiconductor device)

RN 169896-41-7 HCA

CN Tantalum, tris(N-ethylethanaminato) [2-methyl-2-propanaminato(2-)]-, (T-4) - (9CI) (CA INDEX NAME)



IC ICM B32B019-00

NCL 438240000

CC 76-3 (Electric Phenomena)

IT 546-68-9, Titanium tetra-isopropoxide 3087-39-6, Titanium tetrakis(t-butoxide) 3275-24-9, Titanium tetrakis(dimethylamide) 4419-47-0, Titanium tetrakis(diethylamide) 6074-84-6, Tantalum ethoxide 52406-69-6 52406-81-2 **169896-41-7**
172901-22-3 177580-52-8 177580-53-9 238757-13-6

(vapor deposition precursor; method for fabricating gate oxide layer for a semiconductor device)

L23 ANSWER 3 OF 19 HCA COPYRIGHT 2001 ACS

134:260170 Formation of dielectric layer of capacitor. Fuang, Guo Tai; You, Cui Rong (Lien Hua Electronics Co., Ltd., Taiwan). Jpn. Kokai Tokkyo Koho JP 2001085423 A2 20010330, 6 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1999-256379 19990909.

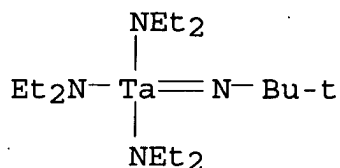
AB The title method involves prep. an org. compd. contg. Ta and an org. compd. contg. Ti, and carrying out MOCVD using the org. compds. as precursors. A dielec. layer of tantalum titanium oxide having a high dielec. const. is formed. A method is also described, for forming a capacitor of a DRAM using the above method.

IT 169896-41-7

(MOCVD of tantalum titanium (oxide dielec. layer of capacitor))

RN 169896-41-7 HCA

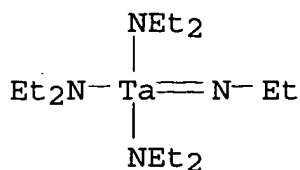
CN Tantalum, tris(N-ethylethanaminato) [2-methyl-2-propanaminato(2-)]-, (T-4) - (9CI) (CA INDEX NAME)



- IC ICM H01L021-316
 ICS C23C016-40; H01L021-31; H01L027-108; H01L021-8242; H01G004-33;
 H01G004-10
- CC 76-10 (Electric Phenomena)
 Section cross-reference(s): 75
- ST **MOCVD** tantalum titanium oxide dielec film DRAM capacitor
- IT Memory devices
 (DRAM (dynamic random access); **MOCVD** of tantalum
 titanium oxide dielec. layer of capacitor)
- IT Capacitors
 Dielectric films
 (**MOCVD** of tantalum titanium oxide dielec. layer of
 capacitor)
- IT Vapor deposition process
 (metalorg.; **MOCVD** of tantalum titanium oxide dielec.
 layer of capacitor)
- IT 60866-78-6, Tantalum titanium oxide
 (**MOCVD** of tantalum titanium oxide dielec. layer of
 capacitor)
- IT 546-68-9, Titanium tetraisopropoxide 3087-39-6 3275-24-9,
 Titanium tetrakisdimethylamide 4419-47-0, Titanium
 tetrakisdiethylamide 6074-84-6, Tantalum pentaethoxide
 52406-69-6 **169896-41-7** 172901-22-3 177580-52-8
 177580-53-9 238757-13-6
 (**MOCVD** of tantalum titanium oxide dielec. layer of
 capacitor)

L23 ANSWER 4 OF 19 HCA COPYRIGHT 2001 ACS

- 134:108338 **MOCVD of tantalum nitride** (Ta_{Nx}, x=0.3-1.5) film.
 Nagano, Kenzo; Nakamura, Satoshi; Komatsu, Takashi; Higuchi,
 Yasushi; Taguma, Yasuhiro (ULVC Japan, Ltd., Japan). Jpn. Kokai
 Tokkyo Koho JP 2001011631 A2 20010116, 4 pp. (Japanese). CODEN:
 JKXXAF. APPLICATION: JP 1999-183563 **19990629** — *not pursuant*
- AB The title method involves using ammonia and a metalorg. precursor
 mixt. of a metalorg. compd. having a Ta=N double bond and a
 metalorg. compd. free of a Ta=N double bond. The tantalum nitride
 film is useful as a barrier film of a semiconductor device.
- IT **67313-80-8**
 (precursors for **MOCVD** of tantalum nitride (Ta_{Nx},
 x=0.3-1.5) film useful for semiconductor device barrier)
- RN 67313-80-8 HCA
- CN Tantalum, [ethanaminato(2-)]tris(N-ethylethanaminato)-, (T-4)- (9CI)
 (CA INDEX NAME)



- IC ICM C23C016-34
ICS H01L021-285
- CC 75-1 (Crystallography and Liquid Crystals)
Section cross-reference(s): 76
- ST **MOCVD** tantalum nitride barrier semiconductor device
- IT Vapor deposition process
(metalorg.; precursors for **MOCVD** of tantalum nitride
(TaN_x , $x=0.3-1.5$) film useful for semiconductor device barrier)
- IT Diffusion barrier
Semiconductor device fabrication
Semiconductor devices
(precursors for **MOCVD** of tantalum nitride (TaN_x ,
 $x=0.3-1.5$) film useful for semiconductor device barrier)
- IT 7664-41-7, Ammonia, uses 67313-80-8 98145-63-2
(precursors for **MOCVD** of tantalum nitride (TaN_x ,
 $x=0.3-1.5$) film useful for semiconductor device barrier)
- IT 12033-62-4, Tantalum nitride (TaN) 12033-63-5, Tantalum nitride
(TaNO_5) 122362-88-3, Tantalum nitride (TaNO_8) 150533-60-1,
Tantalum nitride (TaNO_2) 318522-19-9, Tantalum nitride
($\text{TaNO}_{3-1.5}$)
(precursors for **MOCVD** of tantalum nitride (TaN_x ,
 $x=0.3-1.5$) film useful for semiconductor device barrier)
- L23 ANSWER 5 OF 19 HCA COPYRIGHT 2001 ACS
- 134:94293 Liquid precursor mixtures for deposition of multicomponent metal containing electronic materials. Senzaki, Yoshihide; Roberts, David Allen; Norman, John Anthony Thomas (Air Products and Chemicals, Inc., USA). Eur. Pat. Appl. EP 1067595 A2 20010110, 8 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO. (English). CODEN: EPXXDW. APPLICATION: EP 2000-114321 20000704. PRIORITY: US 1999-350074 19990708.
- AB The process for deposition of a multiple metal or metal compd. layer on a substrate of an electronic material comprises providing a solventless mixt. of .gtoreq.2 metal-ligand complex precursors which constitute a liq. at ambient conditions, in which the ligands are the same and are selected from the group consisting of alkyls, alkoxides, halides, hydrides, amides, imides, azides, nitrates, cyclopentadienyls, carbonyls, and their F, O and N substituted analogs. The solventless mixt. are delivered by direct liq. injection to a flash vaporization zone to vaporize the solventless mixt., and a resulting vapor of the solventless mixt. is contacted with a substrate under deposition conditions to deposit a multiple metal or metal compd. layer on the substrate. Alternatively, the

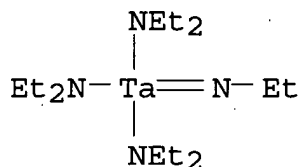
solventless mixt. is delivered to a deposition zone where a substrate is located; and the substrate under deposition conditions is contacted with the solventless mixt. to deposit a multiple metal or metal compd. layer on the substrate. The contacting process on the substrate is selected from the group consisting of **chem** . **vapor deposition**, spray pyrolysis, sol-gel processing, spin coating, and at. layer epitaxy.

IT 67313-80-8

(liq. precursor mixts. for deposition of multicomponent metal contg. electronic materials)

RN 67313-80-8 HCA

CN Tantalum, [ethanaminato(2-)]tris(N-ethylethanaminato)-, (T-4)- (9CI)
(CA INDEX NAME)



IC ICM H01L021-288

CC 76-3 (Electric Phenomena)

Section cross-reference(s): 75

IT **Vapor deposition** process

(**chem.**; liq. precursor mixts. for deposition of multicomponent metal contg. electronic materials)

IT 555-75-9 1071-76-7 1624-01-7 3275-24-9 4419-47-0 5593-70-4
6074-84-6 13801-49-5 14254-05-8 19756-04-8 19824-55-6
19824-57-8 19824-59-0 19824-60-3 25169-05-5 62029-51-0
67313-80-8 70599-04-1 220613-03-6 318277-04-2
318277-05-3 318277-06-4 318277-07-5

(liq. precursor mixts. for deposition of multicomponent metal contg. electronic materials)

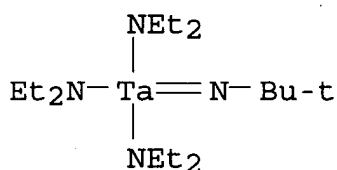
L23 ANSWER 6 OF 19 HCA COPYRIGHT 2001 ACS

134:64030 Metalorganic CVD of tantalum oxide from tert-butylimidotris(diethylamido)tantalum and oxygen. Chiu, Hsin-Tien; Wang, Chun-Nan; Chuang, Shiow-Huey (Department of Applied Chemistry, National Chiao Tung University, Hsinchu, 30050, Taiwan). Chem. Vap. Deposition, 6(5), 223-225 Published in: Adv. Mater. (Weinheim, Ger.), 12(19) (English) 2000. CODEN: CVDEFX. ISSN: 0948-1907. Publisher: Wiley-VCH Verlag GmbH.

AB The results are reported of preliminary exploration of metalorg. CVD of tantalum oxide from tert-butylimidotris(diethylamido)tantalum and oxygen. Tert-butylimidotris(diethylamido)tantalum, (TBTDET) with a higher vapor pressure than Ta(OEt)₅, and other tantalum alkoxides, can be used as a precursor to grow tantalum oxide thin films by CVD for device application. Using this precursor, a Ta₂O₅ film with a thickness of 180 nm had a leakage c.d. below 1 .times. 10⁻⁸ A/cm²

for an elec. field strength of 2 MV/cm, and a breakdown voltage of 2 MV/cm. The dielec. const. was 22.

- IT 169896-41-7, tert-Butylimidotris(diethylamido)tantalum
(metalorg. CVD and elec. properties of tantalum oxide
from tert-butylimidotris(diethylamido)tantalum and oxygen for
device application)
- RN 169896-41-7 HCA
- CN Tantalum, tris(N-ethylethanaminato)[2-methyl-2-propanaminato(2-)]-,
(T-4)-(9CI) (CA INDEX NAME)



- CC 75-1 (Crystallography and Liquid Crystals)
Section cross-reference(s): 76
- ST metalorg CVD tantalum oxide butylimidotrisdiethylamidotant
alum oxygen
- IT Dielectric constant
Electric field
Leakage current
Semiconductor devices
(metalorg. CVD and elec. properties of tantalum oxide
from tert-butylimidotris(diethylamido)tantalum and oxygen for
device application)
- IT Vapor deposition process
(metalorg.; metalorg. CVD and elec. properties of
tantalum oxide from tert-butylimidotris(diethylamido)tantalum and
oxygen for device application)
- IT 1314-61-0, Tantalum oxide Ta₂O₅
(metalorg. CVD and elec. properties of tantalum oxide
from tert-butylimidotris(diethylamido)tantalum and oxygen for
device application)
- IT 7782-44-7, Oxygen, reactions 169896-41-7,
tert-Butylimidotris(diethylamido)tantalum
(metalorg. CVD and elec. properties of tantalum oxide
from tert-butylimidotris(diethylamido)tantalum and oxygen for
device application)

L23 ANSWER 7 OF 19 HCA COPYRIGHT 2001 ACS

133:289409 MOCVD of high-K dielectrics and conductive metal
nitride thin films. Senzaki, Yoshihide; Hamilton, Richard F.; Reid,
Kimberly G.; Hobbs, Christopher C.; Hegde, Rama I.; Tiner, Mike J.
(Schumacher, Carlsbad, CA, 92009, USA). Mater. Res. Soc. Symp.
Proc., 606 (Chemical Processing of Dielectrics, Insulators and
Electronic Ceramics), 13-22 (English) 2000. CODEN: MRSPDH. ISSN:
0272-9172. Publisher: Materials Research Society.

AB A known liq. mixt. of [(CH₃CH₂)₂N]₃Ta=NCH₂CH₃ and

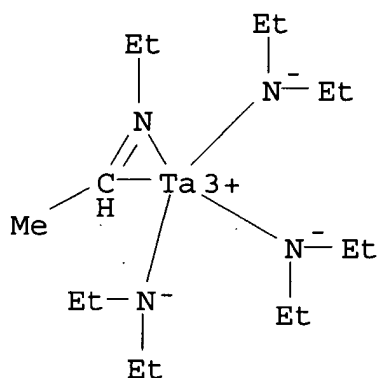
$[(CH_3CH_2)_2N]_3Ta[.eta.2-CH_3CH_2N=CH(CH_3)]$ was studied to deposit Ta_2O_5 and TaN thin films by CVD. Films were deposited at temps. below 400.degree.C using oxygen for oxide and ammonia for nitride, resp. XRD anal. revealed that as-deposited amorphous tantalum oxide films were converted to hexagonal Ta_2O_5 after annealing under oxygen, while tantalum nitride thin films contained cubic TaN as deposited. The low viscosity, thermal stability, and sufficient volatility of the precursor allows direct liq. injection to deliver the precursor, which results in high deposition rate and uniformity of the deposited films.

IT 67296-24-6 67313-80-8 300408-20-2

(MOCVD of high-K dielecs. and conductive metal nitride thin films)

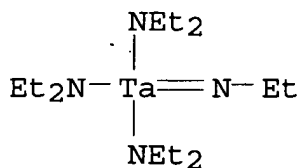
RN 67296-24-6 HCA

CN Tantalum, tris(N-ethylethanaminato)(.eta.2-N-ethylideneethanamine)-(9CI) (CA INDEX NAME)



RN 67313-80-8 HCA

CN Tantalum, [ethanaminato(2-)]tris(N-ethylethanaminato)-, (T-4)- (9CI)
(CA INDEX NAME)



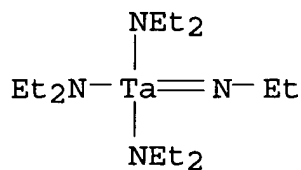
RN 300408-20-2 HCA

CN Tantalum, [ethanaminato(2-)]tris(N-ethylethanaminato)-, (T-4)-, mixt. with tris(N-ethylethanaminato)(.eta.2-N-ethylideneethanamine)tantalum (9CI) (CA INDEX NAME)

CM 1

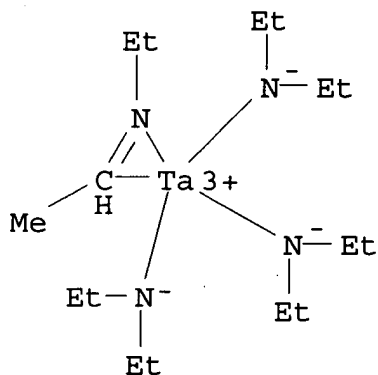
CRN 67313-80-8

CMF C14 H35 N4 Ta
CDES 7:T-4



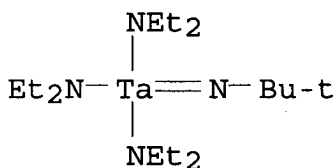
CM 2

CRN 67296-24-6
CMF C16 H39 N4 Ta
CCI CCS



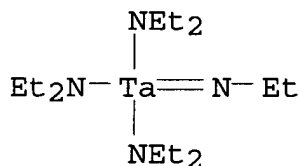
CC 76-3 (Electric Phenomena)
Section cross-reference(s): 75
ST **MOCVD** tantalum oxide nitride film
IT Annealing
Controlled atmospheres
Crystallization
Dielectric constant
Dielectric films
Leakage current
Semiconductor device fabrication
(**MOCVD** of high-K dielects. and conductive metal nitride thin films)
IT Films
(elec. conductive; **MOCVD** of high-K dielects. and conductive metal nitride thin films)
IT Electric conductors
(films; **MOCVD** of high-K dielects. and conductive metal nitride thin films)
IT Vapor deposition process

- (metalorg.; **MOCVD** of high-K dielecs. and conductive metal nitride thin films)
- IT 1314-61-0, Tantalum pentoxide 12033-62-4, Tantalum nitride TaN
(**MOCVD** of high-K dielecs. and conductive metal nitride thin films)
- IT 7782-44-7, Oxygen, processes
(**MOCVD** of high-K dielecs. and conductive metal nitride thin films)
- IT 67296-24-6 67313-80-8 300408-20-2
(**MOCVD** of high-K dielecs. and conductive metal nitride thin films)
- IT 7664-41-7, Ammonia, reactions
(**MOCVD** of high-K dielecs. and conductive metal nitride thin films)
- L23 ANSWER 8 OF 19 HCA COPYRIGHT 2001 ACS
- 133:97909 Formation of copper thin films by **chemical vapor deposition**. Kusumoto, Toshiro; Murata, Masaaki; Ichihashi, Motoko (ULVC Japan, Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 2000195863 A2 20000714, 6 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1998-370603 19981225.
- AB The processes involves depositing TiN or TaN thin films on substrates with barrier metal films by **CVD**, followed with depositing Cu thin films by **CVD**. The raw materials for Cu thin film deposition may be Cu(I) (HFAC)VTMS or Cu(II) (HFAC)2. The raw materials for TiN film may be Ti(NMe2)4, Ti(NEt2)4, and/or Ti(i-PrNMe)4 and the raw materials for TaN may be Ta(NMe2)5 and/or Ta:N(tert-butyl)(NMe2)3. The **CVD**-Cu film have excellent adhesion and smoothness.
- IT 169896-41-7
(formation of copper thin films on substrates with barrier metal films by **CVD**)
- RN 169896-41-7 HCA
- CN Tantalum, tris(N-ethylethanaminato) [2-methyl-2-propanaminato(2-)]-, (T-4) - (9CI) (CA INDEX NAME)

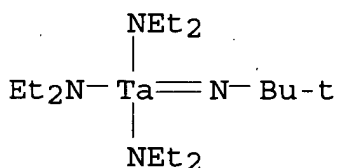


- IC ICM H01L021-3205
- ICS C23C016-18; C23C016-34; H01L021-285
- CC 76-3 (Electric Phenomena)
- ST copper thin film formation CVD underlayer; titanium nitride underlayer copper thin film CVD; tantalum nitride underlayer copper thin film CVD
- IT 7440-50-8P, Copper, preparation
(formation of copper thin films on substrates with barrier metal

- films by CVD)
- IT 3275-24-9, Tetrakis(dimethylamino)titanium 4419-47-0,
Tetrakis(diethylamino)titanium 14781-45-4 19824-59-0,
Pentakis(dimethylamino)tantalum 139566-53-3, Copper(I)
hexafluoroacetylacetonate trimethylvinylsilane 169896-41-7
282107-41-9
(formation of copper thin films on substrates with barrier metal
films by CVD)
- IT 12033-62-4, Tantalum nitride 25583-20-4, Titanium nitride
(thin films, formation of, by CVD; formation of copper
thin films on substrates with barrier metal films by CVD
)
- L23 ANSWER 9 OF 19 HCA COPYRIGHT 2001 ACS
- 132:238802 **Chemical vapor deposition**
process and device manufactured by the method. Machida, Hideaki;
Higuchi, Noboru; Kokubu, Hiroshi; Funakubo, Hiroshi (Tori Chemical
Kenkyusho K. K., Japan). Jpn. Kokai Tokkyo Koho JP 2000087240 A2
20000328, 17 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP
1998-256867 19980910.
- AB The method involves using an org. metal compd. having free groups
and performing vapor transport using a carrier gas contg. a compd.
having the groups or a compd. having the groups as a carrier gas. A
Ca-, Sr-, Ba-, Pb-, Ta-, Cu-, Ti-, Zr-, and Al-based film are
manufd. by the method. Stable vapor transport is performed in the
CVD process with decompn. prevention of the compd.
- IT 67313-80-8 169896-41-7
(film formation by CVD for dielec. devices)
- RN 67313-80-8 HCA
- CN Tantalum, [ethanaminato(2-)]tris(N-ethylethanaminato)-, (T-4)- (9CI)
(CA INDEX NAME)



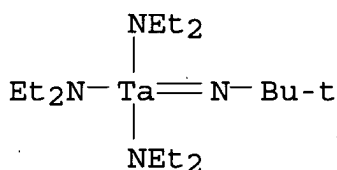
- RN 169896-41-7 HCA
- CN Tantalum, tris(N-ethylethanaminato)[2-methyl-2-propanaminato(2-)]-,
(T-4)- (9CI) (CA INDEX NAME)



- IC ICM C23C016-18
ICS C01G029-00; C23C016-34; C23C016-40; C23C016-448
- CC 47-7 (Apparatus and Plant Equipment)
Section cross-reference(s): 57, 75, 76
- ST metalorg CVD barium strontium titanate dielec; electrode
dielec oxide metalorg CVD; metal nitride film CVD
; vapor transport carrier gas dielec film CVD
- IT Vapor deposition process
(chem.; film formation by CVD for dielec.
devices)
- IT Electric insulators
Electrodes
(film formation by CVD for dielec. devices)
- IT 1304-28-5P, Barium oxide, uses 1305-78-8P, Calcium oxide, uses
1314-11-0P, Strontium oxide, uses 1314-23-4P, Zirconia, uses
1314-61-0P, Tantalum oxide (Ta2O5) 1317-36-8P, Lead oxide (PbO),
uses 7440-50-8P, Copper, uses 12033-62-4P, Tantalum nitride
(TaN) 12058-38-7P, Tungsten nitride (WN) 12673-59-5P, Niobium
Strontium oxide 25583-20-4P, Titanium nitride (TiN) 39427-01-5P,
Aluminum copper oxide 106603-81-0P, Strontium tantalum oxide
(film formation by CVD for dielec. devices)
- IT 64-17-5, Ethanol, processes 75-04-7, Monoethyl amine, processes
75-64-9, tert-Butylamine, processes 109-89-7, processes 112-24-3
112-57-2, Tetraethylene pentamine 124-40-3, Dimethylamine,
processes 598-56-1 754-05-2, Trimethylvinyl silane 1118-71-4
3236-82-6 6074-84-6 7784-21-6, Aluminum hydride 14781-45-4,
Bis(hexafluoroacetylacetonato copper) 16761-83-4 17594-47-7,
Bis(Dipivaloylmethanato barium) 36830-74-7,
Bis(Dipivaloylmethanato strontium) 55161-66-5 59196-92-8
61156-35-2 67313-80-8 118448-18-3,
Bis(Dipivaloylmethanato calcium) 150178-00-0,
Bis(Dipivaloylmethanato lead) 169896-41-7 184675-46-5
245655-35-0 261929-98-0
(film formation by CVD for dielec. devices)
- IT 7440-25-7P, Tantalum, uses 7440-32-6P, Titanium, uses
7440-33-7P, Tungsten, uses
(wiring; film formation by CVD for dielec. devices)
- L23 ANSWER 10 OF 19 HCA COPYRIGHT 2001 ACS
- 132:230668 Method for forming a three-component nitride film containing
metal and silicon for semiconductor device fabrication. Yi,
Kyoung-soo; Koh, Won-yong; Kang, Sang-won (Genitech Co., Ltd., S.
Korea). PCT Int. Appl. WO 2000016377 A2 20000323, 13 pp.
DESIGNATED STATES: W: JP, US; RW: AT, BE, CH, CY, DE, DK, ES, FI,
FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2.
APPLICATION: WO 1999-KR534 19990910. PRIORITY: KR 1998-37257
19980910; KR 1998-48993 19981116.
- AB The method of the present invention comprises the steps of: prepg.
sep. reactive gases each including at least one selected from the
group consisting of a gaseous metal compd., a gaseous Si compd. and
an NH3 gas under conditions such that the gaseous metal compd. and
the NH3 gas does not form a mixt.;. Detg. a sequential gas supply

cycle of the reactive gases so that supplies of the gaseous metal compd., the gaseous Si compd. and the NH₃ gas are each included at least once within one gas supply cycle; and applying the reactive gases to the substrate by repeating the gas supply cycle at least once. According to the present invention, a three-component nitride film can be formed with a uniform thickness despite unevenness of a semiconductor substrate surface.

- IT 169896-41-7, Tris(diethylamido)(tert-butyylimido)tantalum (method for forming three-component nitride film contg. metal and silicon for semiconductor device fabrication)
- RN 169896-41-7 HCA
- CN Tantalum, tris(N-ethylethanaminato)[2-methyl-2-propanaminato(2-)]-, (T-4)- (9CI) (CA INDEX NAME)



- IC ICM H01L
- CC 76-3 (Electric Phenomena)
Section cross-reference(s): 75
- ST **OMCVD** metal nitride silicide film
- IT 3275-24-9, Tetrakis(dimethylamido)titanium 4419-47-0,
Tetrakis(diethylamido)titanium 7664-41-7, Ammonia, reactions
7803-62-5, Silane, reactions 169896-41-7,
Tris(diethylamido)(tert-butyylimido)tantalum
(method for forming three-component nitride film contg. metal and silicon for semiconductor device fabrication)
- L23 ANSWER 11 OF 19 HCA COPYRIGHT 2001 ACS
- 132:29908 Niobium and tantalum derivatives with bidentate nitrogen ligands as potential precursors to nitrides. Hubert-Pfalzgraf, L. G.; Decams, J.-M.; Daniele, S. (Universite Claude Bernard - Lyon I, UMR-CNRS, Villeurbanne, 69622, Fr.). J. Phys. IV, 9(Pr8, Proceedings of the Twelfth European Conference on Chemical Vapour Deposition, 1999, Vol. 2), 953-958 (English) 1999. CODEN: JPICEI. ISSN: 1155-4339. Publisher: EDP Sciences.
- AB Early transition metal derivs. with N-donors have attracted interest as precursors of nitrides, the latter being used as diffusion barriers for the ULSI technol. Potential precursors to niobium and tantalum nitrides were synthesized in good yields and characterized. They are based on bidentate nitrogen donors amidinates, benzamidinates and diamido ligands. These were reacted with niobium or tantalum penta- and tetra-chlorides and TaCl₃(NEt₂)₂. Disubstituted niobium(IV) and tantalum(V) species such as NbCl₂[RNCR'NR₂]₂ [R = Cy, N(SiMe₃)₂; R = SiMe₃, R' = p-tolyl] were obtained and structurally characterized. The more rigid o-dimethylphenylene diamido ligand leads to the volatile, air stable

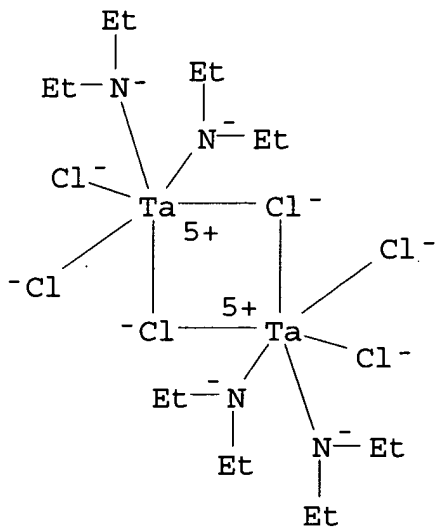
disubstituted Nb(V) species $\text{NbCl}\{\text{N}_2(\text{SiMe}_3)_2\text{C}_6\text{H}_2\text{Me}_2\}_2$. However, π -stacking as shown by x-ray studies are responsible of quite low sublimation rates. Thus, volatility could be reached for some species, their properties, high soly. due to the trimethylsilyl ligands, their stability in soln. is more suited for applications in wet MOCVD than conventional one.

IT 122539-86-0

(for prepn. of tantalum benzamidinato and guanidinato diethylamido chloro complexes as potential nitride precursors)

RN 122539-86-0 HCA

CN Tantalum, di- μ -chlorotetrachlorotetrakis(N-ethylethanaminato)di-, stereoisomer (9CI) (CA INDEX NAME)

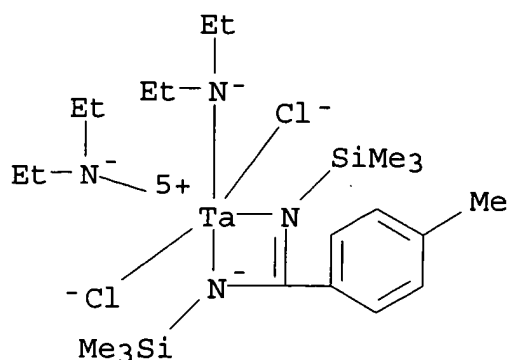


IT 251932-31-7P 251932-32-8P

(prepn. as potential nitride precursor)

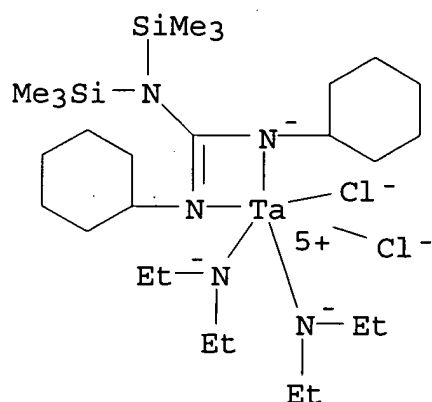
RN 251932-31-7 HCA

CN Tantalum, dichlorobis(N-ethylethanaminato) [4-methyl-N,N'-bis(trimethylsilyl)benzenecarboximidamido- κ .N, κ .N']- (9CI) (CA INDEX NAME)



RN 251932-32-8 HCA

CN Tantalum, dichloro[N',N''-dicyclohexyl-N,N-bis(trimethylsilyl)guanidinato-.kappa.N',.kappa.N'']bis(N-ethylethanaminato)-(9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 75

IT 122539-86-0

(for prepn. of tantalum benzamidinato and guanidinato diethylamido chloro complexes as potential nitride precursors)

IT 251932-29-3P 251932-30-6P 251932-31-7P

251932-32-8P

(prepn. as potential nitride precursor)

L23 ANSWER 12 OF 19 HCA COPYRIGHT 2001 ACS

130:183429 Composite material and its manufacture. Breme, Frank; Guther, Volker; Van Osten, Karl-Uwe (GfE Metalle und Materialien G.m.b.H., Germany). Eur. Pat. Appl. EP 897997 A1 19990224, 15 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO. (German). CODEN: EPXXDW. APPLICATION: EP 1998-115821 19980821. PRIORITY: DE 1997-19736449 19970821.

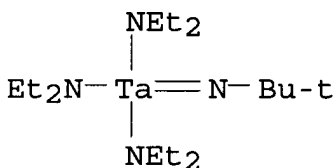
AB The composites comprise a plastic substrate and a deposited continuous layer (thickness $< 2 \mu\text{m}$) of a ductile metal-contg. compd. MaObCxNyBz ($\text{M} = \text{Ti, Ta, Nb, Zr, Hf}$; $a = 0.025-0.9$; $b = 0.025-0.7$; $x = 0.2-0.9$; $y, z = 0-0.7$; $a + b + x + y + z = 1$) such that the M concn. (a) increases continuously from the substrate interface (where a is .apprx.0) to the surface of the deposited layer, and are prep'd. by activating the plastic surface, vapor-depositing an appropriate metal compd. at $\text{ltoreq. } 100^\circ\text{C}$, and treating with a plasma at < 50 millibars. The products find use in medical technol. as prostheses, etc. Thus, poly(ethylene terephthalate) was surface-treated with a 50-W inductive plasma (13.56 MHz) for 3 min at .apprx.1 millibar, heated to .apprx. 100°C , then treated with $\text{Ti}(\text{NMe}_2)_4$ vapors in a H carrier gas stream at 5°C , and exposed to a low-pressure plasma. The coating adhered to the substrate with peel strength $> 6 \text{ N/mm}^2$ and showed cond. $2.1 (\Omega\text{-cm})^{-1}$ initially, which decreased to $0.18 (\Omega\text{-cm})^{-1}$ after 3 days exposure to air.

IT 169896-41-7

(composite material by CVD of)

RN 169896-41-7 HCA

CN Tantalum, tris(N-ethylethanaminato) [2-methyl-2-propanaminato(2-)]-, (T-4) - (9CI) (CA INDEX NAME)



IC ICM C23C016-30

ICS C23C016-18; C23C016-02

CC 38-2 (Plastics Fabrication and Uses)

Section cross-reference(s): 42, 57, 63

ST ceramic thermoplastic composite prosthesis; **chem**
vapor deposition plasma assisted

IT Prosthetic composites

(ceramic-plastic; manuf. of composite materials by CVD)

IT **Chemical vapor deposition**

(in manuf. of composite materials)

IT Plasma

(low-pressure; in manuf. of composite materials by CVD)

IT Fluoropolymers, uses

Polyamides, uses

Polyesters, uses

Polyurethanes, uses

(substrate; composite material by CVD on)

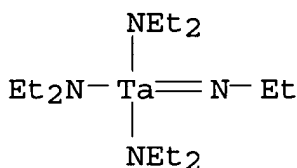
IT 1333-74-0, Hydrogen, uses

(carrier gas; in manuf. of composite materials by CVD)

IT 3275-24-9, Tetrakis(dimethylamino)titanium 19824-58-9,

Pentakis(dimethylamino)niobium 19824-59-0,

- Pentakis(dimethylamino)tantalum 25169-05-5,
 Pentakis(diethylamino)niobium 55161-66-5,
 Pentakis(diethylamido)tantalum **169896-41-7** 210363-27-2
 (composite material by **CVD** of)
- IT 9002-84-0, PTFE 9003-07-0, Polypropylene 25038-59-9,
 Poly(ethylene terephthalate), uses
 (substrate; composite material by **CVD** on)
- L23 ANSWER 13 OF 19 HCA COPYRIGHT 2001 ACS
 129:297190 **CVD** of nitride layers in semiconductor device
 fabrication. Jain, Ajay; Weitzman, Elizabeth (Motorola, Inc., USA).
 Eur. Pat. Appl. EP 869544 A2 19981007, 8 pp. DESIGNATED STATES:
 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, MC, PT, IE,
 SI, LT, LV, FI, RO. (English). CODEN: EPXXDW. APPLICATION: EP
 1998-104865 19980318. PRIORITY: US 1997-829752 19970331.
- AB Refractory metal nitride and refractory metal Si nitride layers can
 be formed by metalorg. **chem. vapor**
deposition. More specifically, TaN can be formed by
CVD using ethyltris(diethylamido)tantalum (ETDET) and NH₃.
 By the inclusion of SiH₄, a TaSiN layer can also be formed. Both of
 these layers can be formed at wafer temps. .ltorsim.400.degree. with
 relatively small amts. of C within the film. The invention can be
 used to form TaN or TaSiN that is relatively conformal and has
 reasonably good diffusion barrier properties.
- IT **67313-80-8**
 (ETDET; in **CVD** of nitride diffusion barrier layers in
 semiconductor device fabrication)
- RN 67313-80-8 HCA
 CN Tantalum, [ethanaminato(2-)]tris(N-ethylethanaminato)-, (T-4)- (9CI)
 (CA INDEX NAME)



- IC ICM H01L021-285
 CC 76-3 (Electric Phenomena)
 Section cross-reference(s): 75
- ST **MOCVD** diffusion barrier semiconductor device; tantalum
 nitride **MOCVD** semiconductor device; silicon tantalum
 nitride **MOCVD** semiconductor device
- IT Diffusion barrier
 (**CVD** of nitride diffusion barrier layers in
 semiconductor device fabrication)
- IT Semiconductor device fabrication
 (**CVD** of nitride layers in)
- IT Refractory metal compounds
 (nitrides; **CVD** of nitride layers in semiconductor

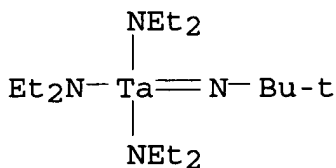
- device fabrication)
- IT Metalorganic **chemical vapor deposition**
(of nitride layers in semiconductor device fabrication)
- IT 12033-62-4, Tantalum nitride 99039-55-1, Tantalum nitride silicide
(CVD of nitride diffusion barrier layers in
semiconductor device fabrication)
- IT 67313-80-8
(ETDET; in CVD of nitride diffusion barrier layers in
semiconductor device fabrication)

L23 ANSWER 14 OF 19 HCA COPYRIGHT 2001 ACS

127:271322 Fabricating a tantalum nitride diffusion barrier for copper
metalization. Sun, Shi-chung; Chiu, Hien-tien; Tsai, Ming-hsing
(United Microelectronics Corp., Taiwan). U.S. US 5668054 A
19970916, 10 pp. (English). CODEN: USXXAM. APPLICATION: US
1996-584749 19960111.

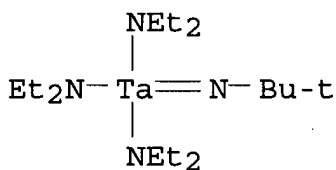
AB A process for fabricating a TaN diffusion barrier for the advanced
Cu metalization of semiconductor devices is disclosed. The process
comprises prepg. a semiconductor device fabricated over the surface
of a Si substrate having a component with a fabricated contact
opening. Before the formation of the Cu contact by deposition, the
process performs a TaN low-pressure CVD procedure that
deposits a TaN film over the substrate. After the Cu deposition, a
photoresist layer is subsequently fabricated for patterning the
deposited Cu contact and TaN layers, whereby the deposited film of
TaN is patterned to form the metalization diffusion barrier for the
semiconductor device. The TaN low-pressure CVD procedure
includes depositing a layer of TaN using the metalorg. precursor
tert-butylimido-tris(diethylamido)tantalum (TBTDET) in a cold-wall
low-pressure reactor with a base pressure of .apprx.10⁻⁵ torr. The
source of the metalorg. precursor is vaporized at
.apprx.40-50.degree.. The typical deposition pressure is .apprx.20
mtorr. A TaN layer of low C content and low resistivity may thus be
formed in the disclosed CVD procedure having effective
capability against Cu diffusion.

- IT 169896-41-7, Tertbutylimidotris(Diethylamido)tantalum
(fabricating a tantalum nitride diffusion barrier for copper
metalization by CVD from)
- RN 169896-41-7 HCA
- CN Tantalum, tris(N-ethylethanaminato)[2-methyl-2-propanaminato(2-)]-,
(T-4) - (9CI) (CA INDEX NAME)



IC ICM H01L021-28
NCL 438653000

- CC 76-3 (Electric Phenomena)
 IT **Chemical vapor deposition**
 (of tantalum nitride diffusion barrier for copper metalization in a semiconductor device)
 IT 169896-41-7, Tertbutylimidotris(Diethylamido)tantalum
 (fabricating a tantalum nitride diffusion barrier for copper metalization by CVD from)
- L23 ANSWER 15 OF 19 HCA COPYRIGHT 2001 ACS
 126:285955 Properties of metalorganic **chemical vapor deposited** tantalum nitride thin films. Sun, S. C.; Tsai, M. H.; Tsai, C. E.; Chiu, H. T. (National Nano Device Laboratory, Institute of Electronics, National Chiao Tung University, Taipei, Peop. Rep. China). Proc. - Int. Conf. Solid-State Integr. Circuit Technol., 4th, 547-549. Editor(s): Baldwin, Gary L. Institute of Electrical and Electronics Engineers: New York, N. Y. (English) 1995. CODEN: 64CRAT.
- AB Low-resistivity Ta nitride (TaN) films were successfully realized by low-pressure metalorg. CVD using a new precursor TBTDET (terbutylimido-tris-diethylamino Ta). Data from TEM and XRD anal. indicated that 600.degree. as-deposited films exhibit the polycryst. structure with <200> preferred orientation. CVD TaN films were studied as diffusion barriers for Cu and Al interconnections.
- IT 169896-41-7
 (starting material; properties of MOCVD tantalum nitride thin films)
- RN 169896-41-7 HCA
 CN Tantalum, tris(N-ethylethanaminato)[2-methyl-2-propanaminato(2-)]-, (T-4) - (9CI) (CA INDEX NAME)



- CC 76-2 (Electric Phenomena)
 Section cross-reference(s): 75
 ST **MOCVD** tantalum nitride film; resistance tantalum nitride film; diffusion barrier tantalum nitride film
 IT Diffusion barrier
 Electric resistance
 Polycrystalline films
 (properties of MOCVD tantalum nitride thin films)
 IT Metalorganic **chemical vapor deposition**
 (properties of MOCVD tantalum nitride thin films)
 IT 7440-44-0, Carbon, occurrence 7782-44-7, Oxygen, occurrence
 (properties of MOCVD tantalum nitride thin films)
 IT 12033-62-4P, Tantalum nitride (TaN)
 (properties of MOCVD tantalum nitride thin films)

IT 169896-41-7

(starting material; properties of MOCVD tantalum nitride thin films)

L23 ANSWER 16 OF 19 HCA COPYRIGHT 2001 ACS

126:164537 Process for the preparation of metal nitride coatings from single source precursors. Winter, Charles H.; Lewkebandara, T. Suren; Jayaratne, Kumudini C. (Wayne State University, USA). U.S. US 5591483 A 19970107, 8 pp. (English). CODEN: USXXAM.

APPLICATION: US 1994-298764 19940831.

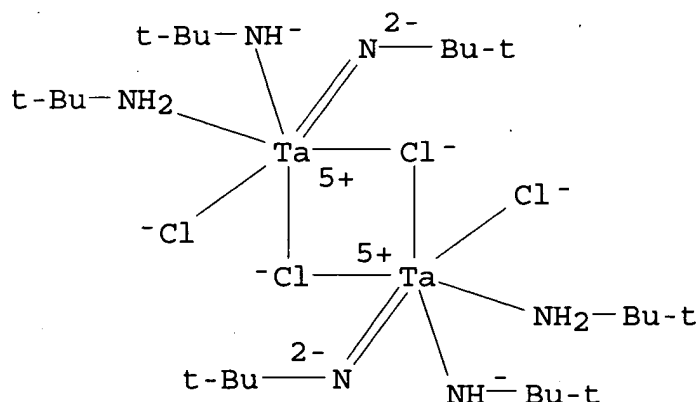
AB Metal nitride coatings are deposited effectively by the decompn. of single source metal imido-amidoamine precursors prep'd. by the reaction of a pentavalent metal halide with a primary amine or hydrazine. Preferably the compds. derived from a pentavalent metal M have the formula $[MCl_2(NR)(NHR)(NH_2R)]_n$, where R is alkyl, cycloalkyl, aryl, cycloalkenyl, or NR_1R_2 , where R_1 and R_2 are independently alkyl, cycloalkyl, alkenyl, cycloalkenyl, aryl, or hydrogen, and where n is a whole no. from 1 to 3, while the compds. derived from a tetravalent metal M' have the formula $[M'Cl_2(NNR_1R_2)(NH_2NR_1R_2)]_n$, where R_1 and R_2 have the same meanings as above, or together with the nitrogen to which they are bonded from a cyclic imine, and where n is a whole no. from 1 to 3, preferably 2. With hydrazine-derived precursors, TaN coatings may be deposited as low as 400.degree. or lower.

IT 90836-77-4P 158990-06-8P

(prepn. as single source precursor for tantalum nitride film deposition)

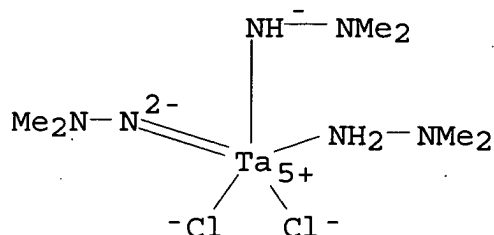
RN 90836-77-4 HCA

CN Tantalum, di-.mu.-chlorodichlorobis(2-methyl-2-propanaminato)bis[2-methyl-2-propanaminato(2-)]bis(2-methyl-2-propanamine)di-, stereoisomer (9CI) (CA INDEX NAME)



RN 158990-06-8 HCA

CN Tantalum, dichloro(1,1-dimethylhydrazinato-N2)[1,1-dimethylhydrazinato(2-)-N2](1,1-dimethylhydrazine-N2)-(9CI) (CA INDEX NAME)



IC ICM C23C016-00

NCL 427248100

CC 75-1 (Crystallography and Liquid Crystals)

ST nitride metal film **CVD** single precursor; tantalum nitride film **CVD** single precursor

IT Nitrides

(**CVD** of metal nitrides using single source precursor)

IT **Chemical vapor deposition**

(of metal nitrides using single source precursor)

IT **90836-77-4P 158990-06-8P**

(prepn. as single source precursor for tantalum nitride film deposition)

L23 ANSWER 17 OF 19 HCA COPYRIGHT 2001 ACS

125:211211 Imido Complexes Derived from the Reactions of Niobium and Tantalum Pentachlorides with Primary Amines: Relevance to the **Chemical Vapor Deposition** of Metal Nitride Films. Jayaratne, Kumudini C.; Yap, Glenn P. A.; Haggerty, Brian S.; Rheingold, Arnold L.; Winter, Charles H. (Department of Chemistry, Wayne State University, Detroit, MI, 48202, USA). Inorg. Chem., 35(17), 4910-4920 (English) 1996. CODEN: INOCAJ. ISSN: 0020-1669.

AB Reactions of NbCl₅ and TaCl₅ with tert-butylamine (.gtoreq.6 equiv) in benzene afford the dimeric imido complexes [NbCl₂(NtBu)(NHtBu)(NH₂tBu)]₂ (90%) and [TaCl₂(NtBu)(NHtBu)(NH₂tBu)]₂ (79%). The Nb complex exists as two isomers in soln., while the Ta complex is composed of three major isomers and at least two minor isomers. Analogous treatments with isopropylamine (.gtoreq.7 equiv) give the monomeric complexes NbCl₂(NiPr)(NH_iPr)(NH₂iPr)₂ (84%) and TaCl₂(NiPr)(NH_iPr)(NH₂iPr)₂ (84%). The monomeric complexes are unaffected by treatment with excess isopropylamine, while the dimeric complexes are cleaved to the monomers MCl₂(NtBu)(NHtBu)(NH₂tBu)₂ upon addn. of excess tert-butylamine in CHCl₃ soln. Treatment of NbCl₅ and TaCl₅ with 2,6-diisopropylaniline affords insol. ppts. of [NH₃(2,6-(CHMe₂)₂C₆H₃)]₂[NbCl₅(N(2,6-(CHMe₂)₂C₆H₃))] (100%) and [NH₃(2,6-(CHMe₂)₂C₆H₃)]₂[TaCl₅(N(2,6-(CHMe₂)₂C₆H₃))] (100%), which react with 4-tert-butylpyridine to afford the sol. complexes [4-t-C₄H₉C₅H₄NH]₂[NbCl₅(N(2,6-(CHMe₂)₂C₆H₃))] (45%) and [4-t-C₄H₉C₅H₄NH]₂[TaCl₅(N(2,6-(CHMe₂)₂C₆H₃))] (44%). Sublimation of

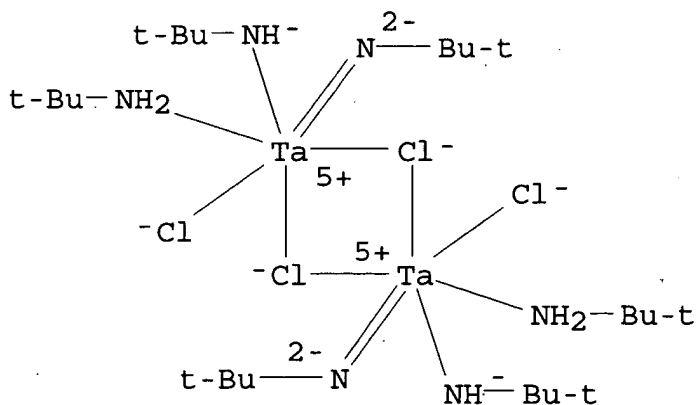
[NbCl₂(NtBu)(NHtBu)(NH₂tBu)]₂, MCl₂(NiPr)(NHiPr)(NH₂iPr)₂, and [NH₃(2,6-(CHMe₂)₂C₆H₃)]₂[MCl₅(N(2,6-(CHMe₂)₂C₆H₃))] leads to disproportionation to give [MCl₃(NR)(NH₂R)]₂ as sublimates (32-49%), leaving complexes of the proposed formulation MCl(NR)₂ as nonvolatile residues. By contrast, [TaCl₂(NtBu)(NHtBu)(NH₂tBu)]₂ sublimates without chem. reaction. Anal. of the org. products obtained from thermal decompn. of [NbCl₂(NtBu)(NHtBu)(NH₂tBu)]₂ showed isobutylene and tert-butylamine in a 2.2:1 ratio. Mass spectra of [NbCl₂(NtBu)(NHtBu)(NH₂tBu)]₂, [TaCl₂(NtBu)(NHtBu)(NH₂tBu)]₂, and [NbCl₃(NiPr)(NH₂iPr)]₂ showed dimeric imido complexes, monomeric imido complexes, and nitrido complexes, implying that such species are important gas phase species in CVD processes using these mol. precursors. [4-T-C₄H₉C₅H₄NH]₂[NbCl₅(N(2,6-(CHMe₂)₂C₆H₃))] crystallizes in the space group P2₁/c with a 12.448(3), b 10.363(3), c 28.228(3) .ANG., .beta. 94.92(1).degree., and Z = 4. [NbCl₃(NiPr)(NH₂iPr)]₂ crystallizes in the space group P2₁/c with a 9.586(4), b 12.385(4), c 11.695(4) .ANG., .beta. 112.89(2).degree., and Z = 2. [NbCl₃(N(2,6-(CHMe₂)₂C₆H₃))(NH₂(2,6-(CHMe₂)₂C₆H₃))]₂ crystallizes in the space group P2₁/n with a 10.285(3), b 11.208(3), c 23.867(6) .ANG., .beta. 97.53.degree., and Z = 2. [TaCl₃(N(2,6-(CHMe₂)₂C₆H₃))(NH₂(2,6-(CHMe₂)₂C₆H₃))]₂ crystallizes in the space group P2₁/n with a 10.273(1), b 11.241(2), c 23.929(7) .ANG., .beta. 97.69(2).degree., and Z = 2. These findings are discussed in the context of Nb and Ta nitride film depositions from mol. precursors.

IT 90836-77-4P 180966-34-1P

(prepn. as CVD precursor and decompn. during attempted sublimation)

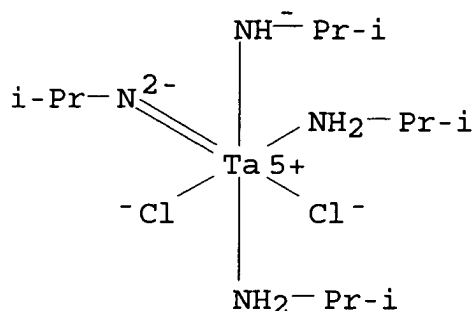
RN 90836-77-4 HCA

CN Tantalum, di-.mu.-chlorodichlorobis(2-methyl-2-propanaminato)bis[2-methyl-2-propanaminato(2-)]bis(2-methyl-2-propanamine)di-, stereoisomer (9CI) (CA INDEX NAME)



RN 180966-34-1 HCA

CN Tantalum, dichloro(2-propanaminato)[2-propanaminato(2-)]bis(2-propanamine)-(9CI) (CA INDEX NAME)

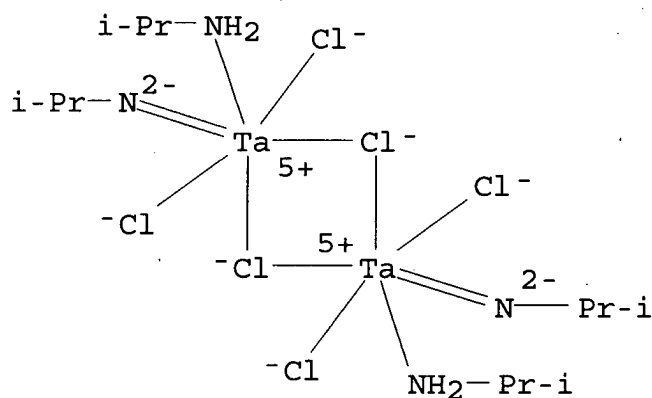


IT 180966-42-1P

(prepn. by decompn. of CVD precursor during attempted sublimation)

RN 180966-42-1 HCA

CN Tantalum, di-.mu.-chlorotetrachlorobis[2-propanaminato(2-)]bis(2-propanamine)di-, stereoisomer (9CI) (CA INDEX NAME)

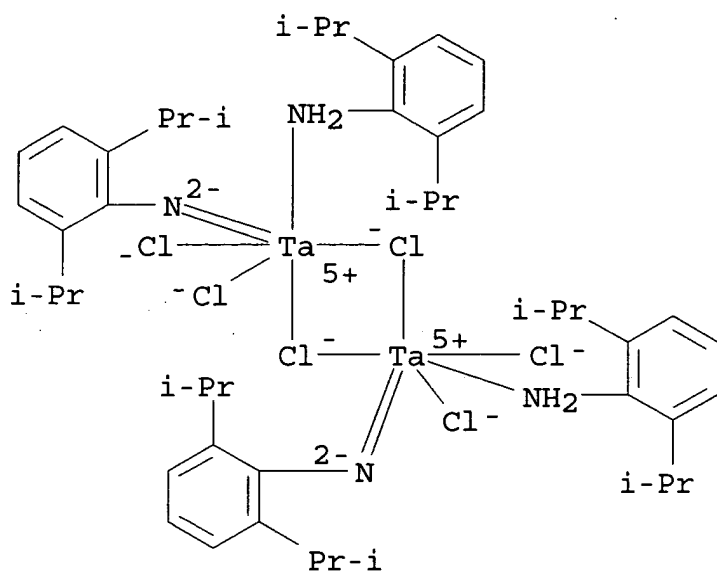


IT 180966-44-3P

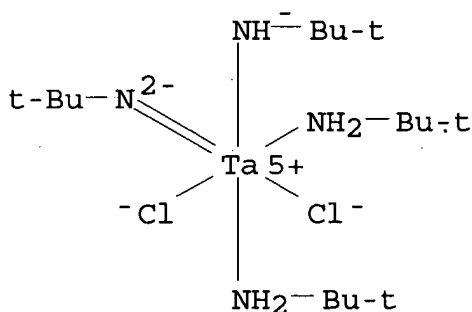
(prepn. by decompn. of CVD precursor during attempted sublimation and crystal structure of)

RN 180966-44-3 HCA

CN Tantalum, bis[2,6-bis(1-methylethyl)benzenaminato(2-)]bis[2,6-bis(1-methylethyl)benzenamine]di-.mu.-chlorotetrachlorodi-, stereoisomer (9CI) (CA INDEX NAME)



IT 180966-48-7P
 (prepn. of)
 RN 180966-48-7 HCA
 CN Tantalum, dichloro(2-methyl-2-propanaminato)[2-methyl-2-propanaminato(2-)]bis(2-methyl-2-propanamine) - (9CI) (CA INDEX NAME)

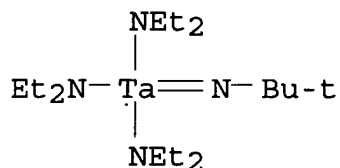


CC 78-9 (Inorganic Chemicals and Reactions)
 Section cross-reference(s): 75
 ST crystal structure niobium tantalum imido chloro; structure niobium tantalum imido CVD precursor; niobium imido chloro prepn CVD precursor; tantalum imido chloro prepn CVD precursor; imido niobium tantalum prepn CVD precursor; thermal reaction niobium tantalum imido CVD; sublimation niobium tantalum imido CVD mechanism; decompn niobium tantalum imido thermal CVD; nitride film niobium tantalum precursor CVD
 IT Sublimation

- (decompn. during attempted sublimation of niobium and tantalum mixed imido amine **CVD** precursors)
- IT Disproportionation
Thermal decomposition
(of niobium and tantalum mixed imido amine **CVD** precursors during attempted sublimation)
- IT Imides
(complexes, niobium and tantalum chloro amine and amide; prepn. as **CVD** precursors and thermal decompn. during attempted sublimation)
- IT Reaction mechanism
(gas-phase, decompn. of niobium and tantalum mixed imido amine **CVD** precursors during attempted sublimation)
- IT 75-31-0, Isopropylamine, reactions 75-64-9, tert-Butylamine, reactions 24544-04-5, 2,6-Diisopropylaniline
(for prepn. of niobium and tantalum imido amido amine chloro complexes as **CVD** precursors)
- IT 10026-12-7, Niobium chloride (NbCl_5)
(for prepn. of niobium imido amine chloro complexes as **CVD** precursors)
- IT 7721-01-9, Tantalum chloride (TaCl_5)
(for prepn. of tantalum imido amido amine chloro complexes as **CVD** precursors)
- IT 115-11-7, Isobutylene, formation (nonpreparative) 180966-46-5
(formation by thermal decompn. of niobium imido amido amine chloro **CVD** precursor)
- IT 180966-39-6P
(prepn. as **CVD** precursor)
- IT 180966-40-9P
(prepn. as **CVD** precursor and crystal structure of)
- IT 90836-77-4P 90836-78-5P 180966-33-0P
180966-34-1P 180966-36-3P 180966-38-5P
(prepn. as **CVD** precursor and decompn. during attempted sublimation)
- IT 180966-42-1P 181141-01-5P
(prepn. by decompn. of **CVD** precursor during attempted sublimation)
- IT 180966-41-0P 180966-43-2P 180966-44-3P
(prepn. by decompn. of **CVD** precursor during attempted sublimation and crystal structure of)
- IT 180966-47-6P 180966-48-7P
(prepn. of)
- L23 ANSWER 18 OF 19 HCA COPYRIGHT 2001 ACS
- 124:329193 Performance of **MOCVD** tantalum nitride diffusion barrier for copper metalization. Sun, S. C.; Tsai, M. H.; Tsai, C. E.; Chiu, H. T. (Department Electronics Engineering, National Chiao Tung University, Hsinchu, Taiwan). Symp. VLSI Technol., Dig. Tech. Pap., 15th, 29-30. Business Center for Academic Societies Japan: Tokyo, Japan. (English) 1995. CODEN: 62PWAR.
- AB A low-resistivity and low C concn. **CVD** TaN film was realized by using a new precursor terbutylimido-tris-diethylamido Ta

(TBTDET). CVD TaN as a diffusion barrier for Cu has higher thermal stability up to 500.degree. than CVD TiN of 450.degree..

- IT 169896-41-7, Tertbutylimido-tris-diethylamido Tantalum
(performance of MOCVD tantalum nitride diffusion barrier for copper metalization)
- RN 169896-41-7 HCA
- CN Tantalum, tris(N-ethylethanaminato)[2-methyl-2-propanaminato(2-)]-,
(T-4)- (9CI) (CA INDEX NAME)



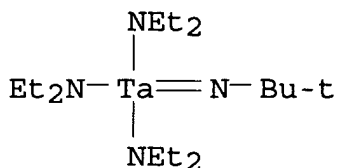
- CC 76-2 (Electric Phenomena)
Section cross-reference(s): 75
- ST MOCVD tantalum nitride diffusion barrier copper;
metalization copper interconnection diode
- IT Diodes
Vapor deposition processes
(performance of MOCVD tantalum nitride diffusion barrier for copper metalization)
- IT Electric conductors
(interconnections, performance of MOCVD tantalum nitride diffusion barrier for copper metalization)
- IT 169896-41-7, Tertbutylimido-tris-diethylamido Tantalum
(performance of MOCVD tantalum nitride diffusion barrier for copper metalization)
- IT 12033-62-4P, Tantalum nitride (TaN)
(performance of MOCVD tantalum nitride diffusion barrier for copper metalization)
- L23 ANSWER 19 OF 19 HCA COPYRIGHT 2001 ACS
- 123:302763 Metalorganic **chemical vapor deposition** of tantalum nitride by tertbutylimidotris(diethylamido)tantalum for advanced metalization. Tsai, M. H.; Sun, S. C.; Chiu, H. T.; Tsai, C. E.; Chuang, S. H. (Institute Electronics, National Chiao Tung University, Hsinchu, 30050, Taiwan). Appl. Phys. Lett., 67(8), 1128-30 (English) 1995. CODEN: APPLAB. ISSN: 0003-6951.
- AB The authors deposited tantalum nitride (TaN) films by low-pressure metalorg. CVD (LP-MOCVD) using a new precursor tertbutylimidotris(diethylamido)tantalum (TBTDET). Strong Ta-N double bond in the precursor preserved the TaN portion during the pyrolysis process. This method has yielded low-resistivity films. It changed from 10 m.OMEGA. cm (deposited at 500.degree.) to 920 .mu..OMEGA. cm (obtained at 650.degree.). The carbon and oxygen concns. were low in the films deposited at 600.degree., as detd. by

XPS. TEM and x-ray diffraction anal. indicated that the as-deposited films exhibited polycryst. structures with the lattice consts. close to the bulk TaN value. The TaN barrier layer was successfully applied as a glue layer for CVD tungsten (W) metalization schemes.

IT 169896-41-7, Tertbutylimidotris(diethylamido)tantalum
(metalorg. **chem. vapor deposition**
of tantalum nitride by tertbutylimidotris(diethylamido)tantalum
for advanced metalization)

RN 169896-41-7 HCA

CN Tantalum, tris(N-ethylethanaminato) [2-methyl-2-propanaminato(2-)]-,
(T-4)- (9CI) (CA INDEX NAME)



CC 76-2 (Electric Phenomena)
Section cross-reference(s): 75

ST metalorg **chem vapor deposition**
tantalum nitride; metalization tantalum nitride metalorg CVD

IT Electric contacts
Vapor **deposition** processes
(metalorg. **chem. vapor deposition**
of tantalum nitride by tertbutylimidotris(diethylamido)tantalum
for advanced metalization)

IT 12033-62-4P, Tantalum nitride
(metalorg. **chem. vapor deposition**
of tantalum nitride by tertbutylimidotris(diethylamido)tantalum
for advanced metalization)

IT 169896-41-7, Tertbutylimidotris(diethylamido)tantalum
(metalorg. **chem. vapor deposition**
of tantalum nitride by tertbutylimidotris(diethylamido)tantalum
for advanced metalization)

=> d his 124-

(FILE 'HCA' ENTERED AT 13:48:44 ON 20 JUN 2001)

FILE 'REGISTRY' ENTERED AT 14:12:06 ON 20 JUN 2001

FILE 'HCA' ENTERED AT 14:13:02 ON 20 JUN 2001

FILE 'LREGISTRY' ENTERED AT 14:15:37 ON 20 JUN 2001

L24 STR

```

L25      0 S L24 SSS SAM SUB=L11
L26      4 S L24 SSS FUL SUB=L11
          SAV L26 PAD859C/A

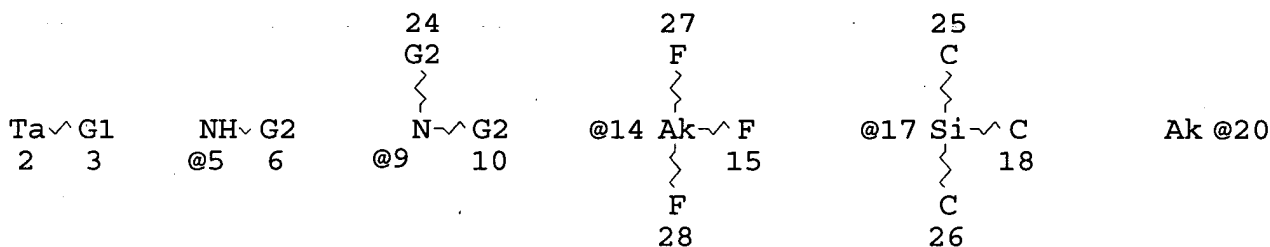
```

```

L27      3 S L26
L28      2 S L27 NOT (L17 OR L22)

```

L9 STR



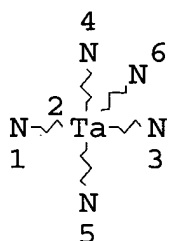
```

NSPEC      IS RC      AT      2
NSPEC      IS RC      AT     18
NSPEC      IS RC      AT     25
NSPEC      IS RC      AT     26
CONNECT    IS E1      RC AT     20
DEFAULT    MLEVEL     IS ATOM
GGCAT      IS SAT      AT     20
DEFAULT    ECLEVEL    IS LIMITED
ECOUNT     IS M1-X4    C      AT     20

```

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 16

```
L11      283 SEA FILE=REGISTRY SSS FUL L9
L24      STR
```



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

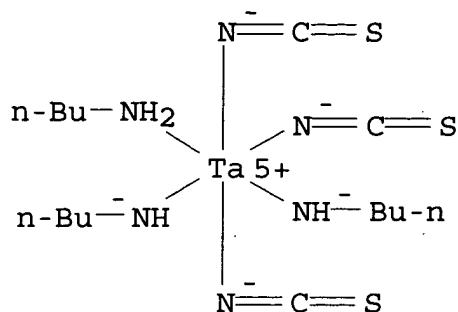
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE
L26 4 SEA FILE=REGISTRY SUB=L11 SSS FUL L24

100.0% PROCESSED 85 ITERATIONS 4 ANSWERS
SEARCH TIME: 00.00.01

=> d l28 1-2 ibib abs hitstr hitind

L28 ANSWER 1 OF 2 HCA COPYRIGHT 2001 ACS
ACCESSION NUMBER: 83:70718 HCA
TITLE: Cyanate compounds and their reactivity. XXI.
Reactivity of niobium(V) and tantalum(V)
thiocyanates to nitrogen donators
AUTHOR(S): Boehland, H.; Harke, E.
CORPORATE SOURCE: Sekt. Chem. Biol., Paedagog. Hochsch. "Theodor
Neubauer", Erfurt-Muehlhausen, E. Ger.
SOURCE: Z. Anorg. Allg. Chem. (1975), 413(2), 102-8
CODEN: ZAACAB
DOCUMENT TYPE: Journal
LANGUAGE: German
AB The preps. of $[\text{MeC}(\text{NH}_2)_2]\text{MX}_6.2\text{MeCN}$ ($\text{M} = \text{Ta}, \text{Nb}$; $\text{X} = \text{Cl}, \text{SCN}$),
 $[\text{M}(\text{NCS})(\text{NC}(\text{NH}_2)\text{Me})_4(\text{MeC}(\text{NH})\text{NH}_2)]_n$, $[\text{M}(\text{NCS})(\text{NH}_2)_2\text{NH}]_x$,
 $[\text{MeC}(\text{NH}_2)_2][\text{M}(\text{NCS})_4(\text{NC}(\text{NH}_2)\text{Me})_2]$, $[\text{M}(\text{NCS})_3(\text{NC}(\text{NHBu})\text{Me})_2(\text{MeC}(\text{NH})\text{NHBu})]$
, and $[\text{M}(\text{NCS})_3(\text{NHBu})_2(\text{BuNH}_2)]$ are reported. The complexes are
characterized by elemental anal., derivatog. measurements, and ir or
visible absorption spectra.
IT 56142-56-4P
(prepn. of)
RN 56142-56-4 HCA
CN Tantalum, bis(1-butanaminato)(1-butanamine)tris(thiocyanato-N)-
(9CI) (CA INDEX NAME)



CC 78-7 (Inorganic Chemicals and Reactions)
 IT 56113-54-3P 56113-56-5P 56113-72-5P 56113-74-7P 56113-75-8P
 56113-76-9P 56113-78-1P 56113-79-2P **56142-56-4P**
 56142-57-5P 56214-94-9P 56214-95-0P 56227-53-3P 58004-49-2P
 (prepn. of)

L28 ANSWER 2 OF 2 HCA COPYRIGHT 2001 ACS

ACCESSION NUMBER: 70:25323 HCA

TITLE: Reactions between acetonitrile and dialkylamido-compounds of titanium, zirconium, and tantalum

AUTHOR(S): Bradley, Donald C.; Ganorkar, M. C.

CORPORATE SOURCE: Queen Mary Coll., London, Engl.

SOURCE: Chem. Ind. (London) (1968), (44), 1521-2

CODEN: CHINAG

DOCUMENT TYPE: Journal

LANGUAGE: English

AB $M(\text{NMe}_2)_x$, where $M = \text{Ta}, \text{Zr}, \text{and Ti}$, were treated with y moles of MeCN to give $M[\text{N}:\text{C}(\text{Me})\text{NMe}_2]_y(\text{NMe}_2)_{x-y}$. The ir spectra of these compds. showed a strong band in the $1577\text{--}87\text{ cm}^{-1}$ region which was attributed to the NCN group of the dimethylaminoacetaldimino ligand, formed by insertion of MeCN in the $M\text{--NMe}_2$ bond. The compds. prepd. and their characteristic ir bands were $\text{Ti}[\text{N}:\text{C}(\text{Me})\text{NMe}_2](\text{NMe}_2)_3$ (I) 1580 , $\text{Ti}[\text{N}:\text{C}(\text{Me})\text{NMe}_2]_2(\text{NMe}_2)_2$ (II) 1577 , $\text{Zr}[\text{N}:\text{C}(\text{Me})\text{NMe}_2]_4$ (III) 1587 , $\text{Ta}[\text{N}:\text{C}(\text{Me})\text{NMe}_2]_4$ (IV) 1585 cm^{-1} . Hydrolysis of these compds. gave Me_2NH and MeCN . Treatment of $\text{Ti}(\text{NET}_2)_4$ or $\text{Zr}(\text{NET}_2)_4$ with MeCN probably gave Et_2NH and $\text{Ti}(\text{N}:\text{C}:\text{CH}_2)_2$ or $\text{Zr}(\text{N}:\text{C}:\text{CH}_2)_2$ although their ir spectra had the characteristic bands at 1560 and 1587 cm^{-1} , resp., assocd. with compds. I-IV.

IT **24980-83-4P**

(prepn. of)

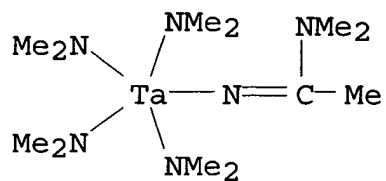
RN 24980-83-4 HCA

CN Tantalum, (N,N-dimethylacetamidinato)tetrakis(dimethylaminato)-, polymers (8CI) (CA INDEX NAME)

CM 1

CRN 45231-66-1

CMF C12 H33 N6 Ta



CC 78 (Inorganic Chemicals and Reactions)

IT 21846-42-4P 21846-44-6P **24980-83-4P** 27081-65-8P

27081-66-9P 27157-35-3P 27157-36-4P

(prepn. of)